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(54) Title: ESTROGEN RECEPTOR LIGANDS

(57) Abstract

Crystal comprising at least part of the ERa ligand binding domain, optionally bound to a ligand, ligands that bind to ER receptors, and methods of designing them, and a homology model of the $\bar{E}R\beta$ receptor.

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Estrogen Receptor Ligands

This invention relates to estrogen receptor ligands. More particularly, the present invention relates to ligands which will bind to estrogen receptors, crystals of such receptors, including crystals of receptor and ligand, synthetic ligands, methods of using such synthetic ligands and methods for designing ligands which will bind to the estrogen receptor.

The thyroid hormone receptor (TR) is known and its three-dimensional structure, and hence its ligand binding domain, has been determined. Knowledge of the three-dimensional structure has enabled a better understanding of the modes of ligand binding and the determination of the optimum conformation of ligand to bind to the receptor. This understanding will provide a pharmacophore model usable in the design of ligands, such as drugs, to bind to the thyroid receptor. It is generally believed in the art that the TR structure also provides a guide to the design of ER ligands.

Estrogen steroid hormone and thus the estrogen receptor (ER) is a member of the steroid hormone receptor family. Its primary natural ligand is estradiol (E2). However, it is known that a large number of structurally diverse non-steroidal compounds such as raloxifene, centchroman, coumestrol, diethylstilbesterol, esculin, tamoxifen, zearalenone, and zindoxifen also bind to the estrogen receptor (Fig. 8). The majority of these non-steroidal estrogen receptor ligands contain 2-4 carboxyclic, aromatic, and/or heterocyclic rings connected by a 1-3 atom chain. One or more of the rings may be fused with the central atom chain or with each other.

It has been proposed that the receptor possesses a multi-functional modular structure potentially having discrete domains for DNA binding, ligand binding, and transactivation. The ligand binding domain (LDB) has been designated domain E and is the largest domain of the estrogen receptor. The ligand binding domain includes a ligand recognition site and regions for receptor dimerzation, interaction with heat

shock proteins, nuclear localization and ligand dependent transactivation.

A review of the structure and functioning of the estrogen receptor is provided in an article by Katzenellenbogen, J. et al., Steroids, (1997) 62(3): 268-303.

It is known that compounds which bind to the estrogen receptor are potentially useful in the treatment a wide range of disease states. These include estrogen agonists for treatment of disease linked to estrogen deficiency (e.g., osteoporosis, cardiovascular and neurodegenerative diseases in post menopausal women) and estrogen antagonists for treatment of breast and uterine cancer. Furthermore, it is known that certain ligands such as tamoxifen display mixed agonist/antagonist action (that is they are either estrogen agonists, estrogen antagonists, or a partial estrogen antagonists when binding to the estrogen receptors of different tissues) and such compounds may simultaneously prevent bone loss and reduce the risk of breast cancer. It is further known that benzothiophenes are usable as agonists or antagonists to steroid hormones, and that it is possible to modify their binding mechanics, for example the binding affinity, by changing the substituent groups at various positions on the molecule. Therefore, it would be desirable to be able to design ligands which are recognizable by and able to bind to the estrogen receptor. Additionally, it would be desirable to know the three dimensional structure of the estrogen receptor. Such knowledge would be useful for the design of compounds intended to bind to the estrogen receptor. The present inventors have been able to produce an estrogen receptor crystal and to determine from that the three dimensional structure of the estrogen receptor. Unexpectedly, the thus determined ER structure reveals that the TR structure does not provide a good model for binding of ligands to ER.

Therefore, in a first aspect the present invention provides an estrogen receptor ligand binding domain crystal.

In a second aspect, the present invention provides ligands, particularly synthetic ligands, of estrogen receptors by use of the crystals.

In a third aspect of the invention, methods for designing ligands which will bind to the estrogen receptor are provided. Such methods use three dimensional models based on the crystals of the estrogen receptor. Generally, such methods comprise, determining compounds which are likely to bind to the receptor based on their three dimensional shape compared to that of the estrogen receptor and in particular the ligand binding domain of the estrogen receptor. Preferably, those compounds have a structure which is complementary to that of the estrogen receptor. Such methods comprise the steps of determining which amino acid or amino acids of the ligand binding domain of the estrogen receptor interacts with the binding ligand, and selecting compounds or modifying existing compounds, to improve the interaction. Preferably, improvements in the interaction are manifested as increases in the binding affinity but may also include increases receptor selectivity and/or modulation of efficacy.

Preferably, the ligands bind to the ER with a high binding affinity, for example within the range of 20-2000 pmol.

The ligands may bind tightly bind to the ER yet not up-regulate gene expression thereby inhibiting the action of estradiol and estradiol mimetics. Thus, the invention also provides a method of inhibiting the activity of estradiol or estradiol mimetics by providing ligands which bind to ER with a high affinity, blocking the activity of estrogens. Alternatively, binding of the ligand to the ER may cause conformational changes to the ER inhibiting further binding thereto. The invention further provides a method of inhibit estradiol activity in an animal, the method comprising administering to the animal a ligand which binds to at least the LBD, of the ER with high affinity and blocks binding of further ligands to at least the LDB of the ER. Such ligands are useful in, for example, the treatment of estrogen receptor mediated diseases in females.

Structure Based Design of ER Ligands

The present work has elucidated the structure of the ligand binding cavity of

the estrogen receptor. Knowledge of the structure of this cavity has utility in the design of structurally novel ER ligands and in the design of non-obvious analogs of known ER ligands with improved properties. These enhanced properties include one or more of the following: (1) higher affinity, (2) improved selectivity for either the α-or β-isoform of the ER, and/or (3) a designed degree of efficacy (agonism vs. partial agonism vs. antagonism). Without knowledge of the ER structure, modifications to produce ligands with enhanced properties and a reasonable likelihood of success would not be available to those skilled in the art. The ER receptor structure also has utility in the discovery of new, structurally novel classes of ER ligands. Electronic screening of large, structurally diverse compound libraries such as the Available Chemical Directory (ACD) will identify new structural classes of ER ligands which will bind to the 3-dimensional structure of the estrogen receptor. Additionally the ER structure allows for "reverse-engineering" or "de novo design" of compounds to bind to the ER.

(1) Enhanced Affinity

The present work has revealed the presence of receptor defined β - and α -face cavities centered respectively above and below the B- and C-rings of estradiol.

The present invention provides new ligands which exploit this discovery by filling the α - and β -face cavities.

Preferably, the ligand fills at least one of the α - and β -face cavities so as to exclude water from the cavity or cavities.

The ligands produced in accordance with the invention bind more effectively to the ER than estradiol. The ligand may bind with twice the binding affinity of estradiol, preferably three times the affinity, and most preferably ten or more times the affinity.

Modifications to the steroid nucleus may be made at the positions marked in R in Fig. 8a and 8b (α -substitution at the 7-, 9-, 12-, 14-, 16-, and 17-positions; β -substitution at the 8-, 11-, 15-, and 18-positions). Preferably, those substituents are hydrophobic substituents, e.g., methyl, ethyl, iso-propyl, chlorine, bromine, or iodine.

Modifications to 2-aryl benzothiophenes may be made at the 2'-, 3'-, and 6'-positions (Fig. 8c) in order to fill the α - and β -face cavities of ER. Preferably substituents should be present in at least two of the following three positions: 3, 2', or 6' so that a perpendicular conformation between the B- and C-rings of the 2-aryl benzothiophene nucleus is enforced. This perpendicular conformation facilitates the positioning of the 2'-, 3'-, and 6'-substituents in the α - and β -face cavities of ER.

In a manner analogous to the benzothiophene series, the affinity of other classes of non-steroidal ER ligands may be enhanced by substitution of small hydrophobic substituents at positions marked R2', R3', and/or R6' in Fig. 8C.

Preferably, the ligand produce in accordance with the invention fills at least one of the α - and β -cavities of the ER without perturbing the remainder of the ER structure.

Another aspect of this invention reveals an unfilled hydrophobic cavity in the raloxifene/ER complex. Filling this cavity with hydrophobic substituents so as to exclude water will enhance binding affinity. This cavity may be filled by positioning a hydrophobic substituent on the ethoxyphenyl sidechain α to the piperidinyl nitrogen atom of raloxifene. This hydrophobic substituent may be a linear alkyl or perfluoroalkyl group (-CH₃ to -C₁₀H₂₁, -CF₃ to -C₁₀F₂₁), benzyl (-CH₂Ph, or methylene cyclohexyl (-CH₂C₆H₁₁).

In a third aspect of this invention, examination of the ER structure reveals that the hydroxyl group at position-3 of estradiol or position-6 of raloxifene form hydrogen bonding interactions with Glu-353 and Arg-394 (Fig. 5a and 5b). It is known that

replacement of the hydroxyl group at position-3 of estradiol or position-6 of raloxifene results in a decrease in affinity for the ER. The invention reveals the reason for this reduction in affinity: while one of the hydrogen atoms of the amino group forms a favorable hydrogen bonding interaction with Glu-353, the second hydrogen atom forms an unfavorable electrostatic interaction with Arg-394. Furthermore this invention reveals a method for enhancing the affinity of 3-amino analogs of estradiol and 6-amino analogs of raloxifene: replacement of one of the two hydrogen atoms of the amino group with an alkyl group to produce a secondary amino group. Alternatively, the amino group may be replaced with a guanidino group (Fig. 8e) which will pick up two additional hydrogen bonding interactions, the first is a salt bridge to Glu-353 and the second is a hydrogen bonding interaction with a backbone carbonyl group in residue Leu-387. Similar enhancement of affinity for the ER may be achieved by replacement of the guanidino group with a fused 2-aminopyrrole (Fig. 8e).

In a closely related aspect of this invention, an understanding is provided for the reduction in affinity for the ER seen in ether derivatives at either position-3 of estradiol or position-6 of raloxifene: electrostatic repulsion between the ether oxygen atom of the ligand and Glu-353 in the ER. This invention reveals a way of increasing the affinity of estradiol position-3 or raloxifene position-6 ether derivatives: replacement of the ether oxygen atom with an amino (NH) group.

In a fourth aspect of this invention, replacement of the 4-hydroxyl group of raloxifene will enhance affinity by picking up a second hydrogen bonding interaction between the amino group and a backbone carbonyl group in Gly-521 of the ER (Fig. 8d).

(2) Improved Selectivity

The estrogen receptor has been found to have two discrete forms, known as $ER\alpha$ and $ER\beta$. Furthermore the ratio of the α - to the β -forms of the ER may vary

considerably in different cell and tissue types. Therefore it may be possible to dissociate desirable therapeutic effects from undesirable side effects of estrogen receptor ligands by designing ligands that selectively bind to one or the other isoforms of the estrogen receptor.

The α - and β -forms of the estrogen receptor differ significantly in their primary sequence and slightly in their tertiary structure. As a consequence of these receptor differences, ligands may bind with different affinity to the two isoforms.

The present inventors have been able to isolate, differentiate and produce crystals for the ER α . From these crystals, the present inventors have determined the three dimensional structure to high resolution. Further, the inventors have created a partial homology model of ER β based on the experimentally derived ER α coordinates. This partial ER β homology model captures the essential differences in binding properties between ER α and ER β . Based on a comparison of the experimental ER α coordinates and the partial homology model of the ER β , the differences between the ER α and ER β have been determined and using these differences, the ability of a ligand to bind to either the ER α and ER β receptors or to both receptors can be predicted. Hence, if it is known that one tissue possesses solely one form of the estrogen receptor, then it is possible to confer a degree of tissue specificity to a ligand by designing the ligand to bind to that predominant form of the receptor. Advantageously, the ligands may be designed to specifically bind ER α ir ER β .

Furthermore, a detailed understanding of the different receptors enables the different behavior of a compound in different tissues to be understood, for example the estrogenic or anti-estrogenic behavior of raloxifen (RAL) dependence on the tissue in which it is active.

Thus, in a further aspect, the invention provides estrogen receptor ligand binding domain crystals for ER α and a partial homology model for ER β . Specificity

of ligands for either the ER α and ER β or even to a specific ratio of ER α to ER β is also provided. The advantage of this is that tissue specificity is conferred to the ligand. Thus, the invention also provides ligands, particularly synthetic ligands of ER α and ER β together with methods for their design.

The present invention provides new ligands which exploit these differences by positioning ligand substituents in close proximity to one or more amino acid residue that differ between the α - and β -isoforms of the ER.

The ligands produced in accordance with the invention bind more effectively to either the α - or β -isoforms of the ER. The selectivity of the binding between the α - or β -isoforms may be ten-fold, more preferably one hundred-fold, and most preferably greater than one thousand-fold.

For example, in the β -face cavity of ER- α , the amino acid residue at position-384 is Leu (sidechain volume = 76.6 Å) whereas in the corresponding position of ER- β , the amino acid residue is Met (sidechain volume = 79.3 Å³). Therefore the β -face cavity of ER- β is smaller. Consequently ER- α selectivity may be enhanced by positioning substituents larger than a methyl group in the β -face cavity in close proximity to residue-384. Interaction between the ligand and residue-384 may be enhanced by introducing substituents at the β 8-. 15-, or 18-positions on the steroid nucleus.

In the α -face cavity of ER- α , the amino acid residue at position-421 is Met (sidechain volume = 79.3 Å³) whereas in ER- β , it is Ile (sidechain volume = 77.3 Å³). Therefore the α -face cavity of ER- α is smaller. This difference may be exploited to produce β -selective compounds through substitutions larger than a methyl group at the α 14-, 16-, or 17-positions of the steroid nucleus.

Similarly, substitutions may be made from either the 2'- or 3'-positions of the 2-arylbenzothiophene nucleus to interact with residue-384 in the β -face cavity or from

the 6'-position to interact with residue-421 in the α -face cavity (Fig. 9a and 9b). However free rotation about the C2-C1' bond will effectively interchange the substituents at the 2'- and 6'-positions thereby reducing selectivity. Moving the hydroxyl group from position-4' (Fig. 9a) to position-5' (Fig. 9b) will bias the binding orientation such that the R_2 substituent will be positioned in the β -face pocket and the R_6 substituent in the α -face pocket. This bias results from the fact that only one of the two possible rotamers about the C2'C1' bond will allow hydrogen bond formation between the 5'-hydroxyl group and the receptor residue His-524.

This invention also provides a means of enhancing the selectivity of other classes of non-steroidal ER ligands. In a manner analogous to the benzothiophene series of ER ligands, substituents larger than methyl may be introduced at either the R2' or R3' positions to produced ER- α selective compounds or at R₆' to produce ER- β selective compounds (Fig. 8c).

Substitutions may be made from position-3 of the steroid nucleus or position-6 of the benzothiophene nucleus to exploit the differences between ER- α and ER- β at position-326 (Ile in ER- α and Val in ER- β) and at position-445 (Phe in ER- α and Tyr in ER- β).

This invention also provides a means for producing specifically ER- α selective ligands. A six atom linker between the hydroxyl group at position-3 of the A-ring of estradiol or at position-6 raloxifene and an aromatic or heteroaromatic ring on the sidechain will position the sidechain ring in close proximity to residue-445 (Fig. 9c). The edge of ER- α Phe-445 and the face of the sidechain ring can form a favorable " π -teeing" interaction. This favorable interaction is not possible with the ER- β Tyr-445, therefore analogs of this type with be ER- α selective (Fig. 9d).

Another aspect of this invention provides a means of further enhancing ER- α selectivity. Introduction of a carboxylate or amino group on the meta or para position of the above mentioned aromatic or heteraromatic ring will form a hydrogen bonding

interaction between the conserved Glu-323 or Lys-449 (Fig. 9e). Alternatively, the heteroaromatic ring may be a pyridone ring which will simultaneously form favorable hydrogen bonding interactions with both Glu-323 or Lys-449 (Fig. 9f). Either of the amino. carboxylate, or pyridone ring substitutions will reinforce the favorable " π -teeing" interaction between the aromatic or heteroatomic ring of the ligand and Phe-445 in ER- α .

(3) Modulation of Efficacy

This invention provides an understanding of the differences between estrogen and antiestrogen binding and therefore a means to design ER ligands with the desired degree of efficacy. An examination of the differences between the ER/estradiol and ER/raloxifene complexes reveals a large movement in Helix-12 (H12, Fig. 6). H12 adopts an "agonistic" conformation defined by the structure of the ER/estradiol complex and an "antagonistic" conformation defined by the structure of the ER/raloxifene complex. These two conformation are in thermodynamic equilibrium. When the ER is complexed with a full agonist, such as estradiol, the equilibrium lies far in the direction of the "agonistic" conformation. In contrast, while when complexed with an antagonist, the equilibrium is pushed in the direction of the "antagonistic" conformation. In the case of raloxifene, the large sidechain at position-3 sterically collides with H12 in it's agonistic conformation, thereby driving the equilibrium strongly in the antagonistic direction. By introduction of progressively shorter sidechains at position-3 of raloxifene, the equilibrium will be gradually shifted back towards the agonist conformation. Thus, this invention provides a means of developing ligands with the desired degree of efficacy (agonist, partial agonist, or antagonist).

In particular, the importance of H12 has been determined as playing a central role in determining the efficacy (agonism vs. antagonism) of a ligand. Thus, ligands which are able to bind to and/or alter the conformation of H12 are of particular importance when designing a ligand or assessing the binding of a ligand, for the

estrogen receptor.

The present inventors have also found the reason why raloxifene has a different binding conformation to that of estradiol, the distinction lying in its active conformation but being unpredictable by virtue of it antagonistic action. The antagonism has been shown, by the present inventors, to be caused by a protruding portion on the raloxifene molecule which causes a large displacement of H12 relative to its conformation in the ER/estradiol complex.

Additionally, it has been found that at least the majority of such receptor proteins are in the form a dimer. Such dimerization leads to a potential route for disruption. Disruptions of this type can be used to predict antagonism or to produce antagonists. Disruptions may take the form of ligand binding which alters the conformation of the helices that comprise the dimerization interface or direct binding to the dimerization interface which then inhibits dimerization.

Further, the orientation of the ligand may be keyed to the receptor, in the dimeric or monomeric form. Furthermore, using the crystals of the present invention, the influence of ligand binding to the LDB on the receptor conformation can now be shown to have influences on the behavior of the receptor since it may disrupt the binding of co-activator, co-repressor, or heat-shock proteins. Previously, such predictions could not me made.

Production of estrogen receptor crystals and their application.

Preferably, the crystal is produced from a sequence comprising at least one hundered and fifty amino acids of the selected estrogen receptor. More preferably, the sequence comprises at least two hundred amino acids. Most preferably, the sequence comprises at least two hundred and fifty amino acids. Preferably, the sequence comprises at least a portion of the ligand binding domain of the estrogen receptor.

More preferably, the sequence comprises the whole ligand binding domain of the estrogen receptor.

Typically ER LBDs are purified to homogeneity for crystallization. Purity of ER LBDs is measured with SDS-PAGE, mass spectrometry, and hydrophobic HPLC. The purified ER for crystallization should be at least 97.5% pure, preferably at least 99.0% pure, and most preferably at least 99.5% pure.

Preferably, the crystals used can withstand exposure to X-ray beams used to produce the diffraction pattern data necessary to solve the X-ray crystallographic structure. For example, crystals grown using estrogen receptor sequence bound to a various of ER ligands have been found to decompose during exposure to X-ray beams at room temperature, whereas crystals grown using estrogen receptor sequence bound to various ER ligands are freezable and are able to withstand exposure to X-ray beams.

Advantageously, the crystals have a resolution determined by X-ray crystallography of less than 3.5 Å and most preferably less than 2.8 Å. Preferably crystals grown using naturally occurring estradiol have an effective resolution of lower than 3.1 Å and crystals grown using raloxifene have an effective resolution of lower than 2.6 Å.

The production of such crystals has enabled the three dimensional structure of the ligand binding domain of the estrogen receptor to be mapped. Use of such crystals in conjunction with the map enables a better understanding of how estradiol and other estrogen bind to the estrogen receptor with precision. This technique can also enable the design of estrogen antagonists since the binding site is known.

For example, in the prior art it has been proposed (see Grease et al., J. Med. Chem. (1997), 40:146-147) to prepare raloxifene analogues using a number of substitutions to the 2-aryl group, one of which is 2-napthyl and shows efficacy in

preventing bone loss at the expense of a loss of binding affinity using, for example a 4'-OH substituent (resulting in a slight affinity loss compared to just a napthyl). Having mapped the estrogen receptor, upon reviewing Formula X below, the fit of such a compound into the estrogen binding site comes intuitively apparent, that is, an amalgamation of the D-ring of estradiol and the pendant position-2 aryl substituent, but using the map, the present inventors have found that a 6'-OH, or even a 5'-OH will be more favorable for affinity.

For example, use of such methods has allowed the present inventors to determine the different binding modes of different steroid hormones to the estrogen receptor such as how the binding of testosterone to the estrogen receptor, which is imperfect binding, differs from that of estradiol. In particular, such models show that there is (1) electrostatic repulsion between the C-3 carbonyl oxygen atom of testosterone and the carboxylate of Glu-353 and (2) steric repulsion between the side chain of the C-18 methyl group of testosterone and the side chain of Leu-387 which accounts for the much lower affinity of testosterone compared to estradiol for the estrogen receptor. The steric hindrance and other stereochemical features of molecules has been found to affect the flexibility, that is the ability to alter the tertiary structure, of the ligand binding domain which therefore affects the perturbility of the ligand binding domain. Therefore, using the crystals of the present invention it is now possible for it to be clearly seen how estradiol binds to the estrogen receptor and hence the structural reasons why a compound behaves as an estrogen can not only be understood but also predicted. This enables an understanding of the promiscuity of the estrogen receptor - its ability to bind a variety of structurally diverse ligands. This understanding can be applied to a greater or lesser extent to all steroid hormone receptors, especially the glucocorticoid receptor.

Crystals of the estrogen receptor binding domain can be used as models in methods for the design of synthetic compounds intended to bind to the receptor. Such models show why very slight difference in chemical moieties of a ligand potentially have widely varying binding affinities. Hence, the three dimensional structure of the

ligand binding domain can be used a pharmaceutical model for compounds which bind to estrogen receptors.

Embodiments of the invention will now be described in more detail, by way of example only, with reference to the accompanying drawing Figure 1 to 23 of which:

Figure 1a shows representative portions of a 2.6 Å resolution multicrystal averaged map for a RAL-ER-LBD complex;

Figure 1b is a 3.1 Å resolution six-fold averaged map for a E2-ER-LBD complex. In both Figure 1a and Figure 1b, the map is contoured at 1F and superimposed on the final, refined models;

Figure 2a is a schematic representation of the ER- LBDa indicating the locations of the various secondary structural elements " and 3₁₀ helices are coloured grey, extended regions are very light grey and coil regions are coloured in dark grey. E2 is coloured very dark grey and is highlighted in space-filling form;

Figure 2b is a topology diagram for ER-LBD. Helices are represented as rectangles and β strands as arrows. The central core layer (H5,H6,H9 and H10 - striped) is sandwiched between the outer flanking layers (H1-4) (H7, H8,H11). The structural elements which flank the layered motif (S1/S2 and H12) are S1, S2, H12 and are cross hatched. The N and C termini are also labelled. All secondary structural elements have been numbered in keeping with the nomenclature that has been established for other known nuclear receptor LBDs;

Figure 3a is a stereoview of the ligand binding cavity. The cavity is viewed in a similar orientation to that given in Fig. 1a. Sidechains for residues that line the cavity are illustrated. Hydrophobic residues are shown in grey, basic residues are shown as spotted and acidic residues are shown in hatched. E2 is coloured black (core) and

dark grey (terminal hydroxyl groups);

Figure 3b is a schematic representation of the ligand binding cavity. Residues that make direct hydrogen bonds to the hydroxyl radius are shown in ball-and-stick representation along with hydrophobic residues that make non-polar interactions with E2 (shown as grey with radial spokes). The atom names and ring nomenclature of E2 are also given;

Figure 3c is a representation of the molecular volume of E2 (dark grey dotted surface) and the accessible binding cavity volume (light grey dotted surface);

Figure 4a is a schematic representations of the ER-α LBD non-crystallographic dimer viewed perpendicular to the dimer axis. The N and C termini are labelled;

Figure 4b is a view of the dimer of Fig. 4a along the dimer axis. E2 is highlighted in mid grey in space-filling form. Helices that are involved in the dimer interface are labelled;

Figure 4c is a view showing the H11 helices that form the backbone of the dimer interface. Interacting residues are show coloured according to polarity (grey -hydrophobic residues; hatched - polar residues; cross-hatched - basic residues);

Figure 5a is a schematic representation of the binding cavity and interactions made by E2. The figure was produced using LIGPLOT software;

Figure 5b is a comparison of the E2 and RAL binding modes (E2 - dark grey; RAL - light grey);

Figure 6 is a schematic representation of the ER-LBD showing the different positioning of helix 12 in the E2 (cross-hatched) and RAL (hatched) complexes. The remainder of the ER-LBD is shown in grey. Dashed lines indicate unmodelled regions

of the structure. The helices which interact with H12 in the two complexes are marked; and

Fig. 7 is a space filling representation of a) an E2 complex and b, an RAL complex. H12 (black) is positioned over the hormone binding cavity in the E2 complex. Raloxifene induces a conformational change so that H12 occupies a hydrophobic groove between H3 and H5. The hydrophobic sidechains of all residues that lie between residues 354 (H3) and 380 (H5) are drawn in dark grey. Other highlighted residues are Lys362 (hatched), Glu380 and Tyr537 (cross-hatched), Asp351 (spots) and the ligand RAL (grey). The remaining atoms of the LBD monomer are white. Note that differences in other parts of the ER-LBD complexes may be due regions missing from the current models;

Fig. 8 shows the structure of several representative estrogen receptor ligands;

Figs. 8a, 8b and 8c show modifications made to the steroid nucleus of ligands which bind to the estrogen receptor;

Figs. 8d and 8e show how affinity of the ligand can be enhanced by adding substituents; and

Figs. 9a-9f show selectivity enhancement by using different substituents on the estrogen receptor ligand; and

Figs. 10 to 19 show by way of structural formulae the chemical reactions involved in the following Examples 1 to 51, which are non-limiting and given by way of illustration only.

Figure 20 shows crystal coordinates for estrogen receptor alpha (ER α) binding domain in complex with raloxifene.

Figure 21 shows crystal coordinates for estrogen receptor alpha (ERa) binding domain in complex with 17-beta-estradiol.

Figure 22 shows a homology model of estrogen receptor alpha (ER α) beta complexed with raloxifene.

Figure 23 shows a homology model of estrogen receptor-beta (ER β) complexed with estradiol.

EXAMPLE 1

Materials

Protein purification and crystallisation of the oestrogen receptor α

The human EP-LBD-α was over expressed in Escherichia coli. (Hegy G.B. et al Steroids (1961 61 June 367-373). Fermentation was carried out as batch and fed batch cultivation in a defined glycerol/salt medium at 30°C. Production of recombinant protein was induced by raising the temperature to 39°C. After 2 h, cells were harvested by centrifugation, and frozen, thawed cells were disrupted by a Bead Beater homogenizer (6 x 22 sec., with a 3 min resting time between bursts) (Biospec. Bartlesville, OK, USA), at 0°C, in 100 mM Tris-HC1 (pH 7.8), 100 mM KC1, 10% glycerol, 4mM EDTA, 4 mM DTT, 5µg/ml antipan. For a fermentation volume of 1200 ml, 250 ml buffer was used with 210 ml acid washed glass beads (212-300 microns). After centrifugation, the supernatant was applied to a column of estradiol-Sepharose Fast Flow, 25 ml, (Greene G. et al Proc Natl Acad Sci USA (1980) 77,5115-5119. The column was first washed with 130 ml 10 mM Tris-HCl. (pH 7.8), 700 mM KC1, 1 mM EDTA, followed first by 130 ml 10 mM Tris-HC1 (pH 7.8), 250 mM NaSCN, 10% dimethyl-formamide, 1 mM EDTA and then by 110 ml 10 mM Tris-HC1 pH 8.0. Reactive Cys residues were modified by washing the column with 120 ml 30 mM Tris-base, 15mM iodoacetic acid, pH 8.1. Excess reagent was washed out by 50 ml Tris-base, 15 mM iodoacetic acid, pH 8.1. Excess reagents was washed

out by 50 ml 10 mM Tris-HC1 pH 8.0 followed by 20 ml 10 mM Tris-HC1, ph 7.8, 250 mM NaSCN, 10% dimethylformamide, 1 mM EDTA. The ET-LBD-α was eluted by including 100 μM of the desired ligand to the last buffer. The fractions containing ER-LBD-α was pooled (65 ml) and concentrated (Centriprep 30, Amicon) to 4 ml. Final purification was achieved using a Bio-Rad 491 preparative PAGE instrument according to the user manual. Using one dilution of the Ornstein/Davies buffer system. The stacking (0.7 cm) and resolving (70 cm) gels was 5.6% (acrylamide/bis). The elution buffer was 10mM Tris-HC1 pH 8.0 and the electrophoresis was carried out at 12 W. Fractions containing ER-LBD-α was pooled and concentrated (Centriprep 30) to the desired protein concentration.

Data collection, phasing and refinement

ER-LBD- α -RAL complex:

A native dataset was collected from a single frozen crystal on beamline X11 at the DESY/Hamburg (1=0.905Å). Diffraction data were recorded at 120K with a 30cm Mar Research image plate located at a crystal-to-detector distance of either 245mm or 390mm. Heavy atom derivatives were collected in-house (York) from flash frozen Data were integrated and reduced using the programs DENZO and SCALPACK. MIR analysis was performed using the CCP4 suite of programs (Table 2). Diffraction data for the alternate C2 (York) and C2221 (DESY, Hamburg) crystal forms were collected to resolutions of 3.0Å and 3.1Å respectively. Initial phases were 3Å using MLPHARE and subsequent two-fold averaging, non-crystallographic matrix refinement and phase extension were carried out using DM. An initial polyalanine trace was used to generate a dimeric search model, using the refined non-crystallographic symmetry and correctly positioned in the alternate C2 and C2221 crystal forms using molecular replacement (AmoRe) Collaborative Computational Project No. 4. (The CCP4 Suite: programs for protein crystallography. Acta Cryst D50, 760-763 (1994)). Twenty cycles of cross crystal averaging between all three crystal forms was carried out with DMMULTI (Supra and Cowtan, K, dm: An automated procedure for phase improvement by density modification. In Joint CCP4 and ESF-EACBM Newsletter on Protein Crystallography 31 PP 34-38 (1994)) using only the MIR phase information. The resultant electron density maps showed no bias towards the input model and enabled the unambiguous tracing of the remainder of the molecule and the assignment of most of the amino acid sequence. Refinement was performed with REFMAC using bulk solvent and anisotropic scaling (.Murshudou et al Acta Cryst D53, 240-255 (1997)). Tight non-crystallographic restraints were maintained during the initial cycles but were loosened in the final stages of refinement. Individual atomic temperature factors were refined isotropically. Residues Asp332, Phe337, Lys416, Lys467, Ser468, Leu469, Glu470 and Glu471 were poorly resolved in the electron density maps and not modelled beyond their C \$ atoms.

ER-LBD- α -E2 complex:

Diffraction data were collected at room temperature from a single ER-LBD-E2 crystal using an 128cm Mar Research image plate located at a crystal-to-detector distance of 280mm on beamline BW7AB at the DESY/Hamburg (l=0.916Å). Initial phase estimates were obtained with AMoRe using the refined ER-LBD RAL dimer (truncated after Met528) as a search model. All data between 15 and 4Å were used for the rotation and translation functions and in the cross-rotation function model Patterson self-vectors were selected within a radius of 30Å. The correct solution, corresponding to three ER-LBD dimers, had a correlation coefficient of 69.8 and an R-factor of 40.6 after AMoRe rigid-body refinement. Six-fold averaging was performed using DM and the structure was refined with REFMAC using tight non-crystallographic restraints, bulk solvent and anisotropic scaling and averaged phases from DM. A single, overall B value was applied in the early stages of refinement until the Rfree converged. Subsequent cycles employed tightly constrained, full isotropic B value refinement. All model building was carried out using the graphics package QUANTA (Molecular Simulations, Inc. San Diego). The sidechains of Leu306, Leu466, Leu 469, Lys492, Lys531 and Leu346 were poorly resolved in the electron density maps and not modelled beyond their C \$ atoms.

TABLE 1

Data collection and refinement statistics

	ER-raloxifene	ER-estradiol
Space group	C2	P21
Unit cell dimensions		
a (Å)	104.53	61.48
B (Å)	53.68	115.16
C (Å)	102.71	137.38
β (ο)	116.79	103.01
No. of molecules / AU	2	6
Resolution (Å)	25 - 2.6	20 - 3.1
No. unique reflections	15,497	34,025
Completeness (%)	94.6	99.1
Multiplicity	4.5	2
Rsym (I)	8	10
Reflections used in	13,868	30,583
refinement		
Rcryst	23.98	22
Rfree	30.4	25.3
Non H atoms	3,741	11,508

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Water	66	126
% A.B,L (a,b,l,p)	92.4 (7.6)	93.0 (7.0)
Rmsd bond length (Å)	0.01	0.01
Rmsd bond angle (Å)	0.04	0.03
Average B protein (Å2)	48.3	37.8
Rmsd NCS protein (Å)	0.57	0.08
Rmsd NCS B (Å2)	8.2	1.1

Rsym (I) = $100x G_hG_i1G_{hi}$ -<I> $>1/G_hG_iI_{h.i}$ where I is the observed intensity. <I> is the average intensity of multiple observations of symmetry related reflections.

Recryst = $100 \times E11F_01-1F_011/E1f_01...$

Rfree is the same as Rcryst but was calculated using a test set of reflections (10% of the whole dataset) that was excluded from the refinement process.

R.m.s. deviation in bond length and the angle distances from Engh and Huber ideal values

R.m.s. distance between all non-crystallographic symmetry (NCS) related atom positions

R.m.s. difference between all non-crystallographic symmetry (NCS) related atomic temperature factors.

TABLE 2
Heavy atom data collection and MIR statistics

Dataset	PCMBS-1	PCMBS-2	KAuCN
Resolution (Å)	20 -3	20 -3	20 -3.6

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No. unique reflections	10,335	9,316	5,835
Completeness (%)	97.6	89	94.2
Multiplicity	4	3.1	2.5
Rsym (I)	8.1	9.2	7
Conc. reagent (mM)	4	4	4
Soak time (days)	5	14	2
Resolution (Å)	20 -3	20 -3	20 -3.6
Riso	16.9	20.7	13.7
No. of sites	2	2	1
Cullis R (centric / acentric)	0.75/0.68	0.76 / 0.66	0.90 / 0.85
Phasing power (centric / acentric)	1.22 / 1.88	1.23 / 2.02	0.71 / 0.94
F.O.M (20 - 3Å) (centric / acentric / overall)		0.67 / 0.48 / 0.49	·

Cullis R =E1E1/G11F_{PH} 1-1FP_P11 for centric (c) and acentric (a) reflections. F.O.M = $\langle EP(\alpha)e^{i\alpha}/EP(\alpha)\rangle$ where α is the phase and $P(\alpha)$ is the phase probability distribution. Phasing power.

EXAMPLE 2

ER -E2 crystallisation

Prior to crystallisation protein was buffer exchanged to 20 mM using Tris/HC1 buffer at pH 7.8 and concentrated to 12-13 mg/ml. Crystals were grown by vapour diffusion using hanging and sitting drop techniques. The best crystals were obtained using 2.4 M Ammonium formate or 80-90 mM Magnesium formate as precipitants buffered with 0.1 M Tris/HC1 buffer. 4 M Ammonium formate or 200 mM Magnesium formate unbuffered stock solutions were used. Magnesium formate stock solution was kept at 4°C and filtered before use. The optimum pH ranged from 7.9 to 8.3 with the best crystals growing at pH 8.1. Protein concentration in the drop was 8 mg/ml although X-ray suitable crystals were also obtained at 13 mg/ml. However, crystals obtained from such conditions were very often twinned and the addition of DMSO at up to 8% significantly improved their quality. The size of the crystals was correlated with the size of the sitting/hanging drop. The optimum size of the drop was achieved by mixing 2.5 ml of protein with 2.5ml of the reserved solution. All crystallisations were performed at 18°C. The best crystals, with a size of 0.5x0.05x0.05 mm³, were mounted in the X-ray quartz capillaries.

ER-α-Raloxifen (ER-R) crystallisation

After purification as before, the protein buffer was replaced with 20 mMTris/HCl pH 7.8-7.9 and the protein was concentrated usually to 10-12 mg/ml. The vapour diffusion method with the hanging drop technique was used for crystallations. The best conditions for crystallisation used the following medium: 0.1 M Tris/HCl buffer pH 8.3, 12% (w/v) of PEG 4000, 0.1 M Maltose, 50 mM Lysine, 0.2 M MgCl2, 5% dioxane. The concentration of the protein solution used for crystallisation was brought up to 7.3-7.5 mg/ml by dilution with 20 mM Tris/HCl buffer pH 8.3. Cyrstallisations were performed with different drop sizes and protein-to-reservoir buffer ratios. The

best crystals were grown from drops obtained by mixing 2 ml of protein with 2 ml or 3 ml of well buffer. The best temperature for crystal growth is 18°C. These conditions yielded the main C2 crystal form (a=104.53Å b=53.68Å c=102.71Å b=116.79Å, in the shape of monoclinic plates (0.1x0.1x0.02 mm³)), which was subsequently used for heavy atoms derivatives searches and structure refinement.

By subtle manipulation of the above conditions other crystal forms were also produced. The lowering of the PEG 4000 concentration to 10-11 % w/v resulted in other C2 crystal form: a=89.9Å b=75.09Å c=87.50Å b=103.01o. These crystals grow at 18°C as single pyramids and despite their severe twinning it was possible to separate mechanically small untwinned fragments of the crystals suitable for X-ray data collection.

The alteration of other conditions, for example increase of dioxan concentration from 5 to 7.5 and 10% and replacement of 50 mM Lys by 50 mM Arg, 0.1 M Maltose by 0.1 M Sucrose or Glucose, produced C2221 orthorhombic crystal form: a=65.47Å b=95.99Å c=164.14Å Crystals reached the size of 0.2x0.03x0.03 mm3 and they were growing preferably at 18°C.

It is also possible to obtain crystals of SeMet derivative or ER-R complex. They can be grown from conditions typical for the main C2 crystal form, but the concentration of dioxan is raised usually up to 7.5%. These crystals were very fragile and give poor quality X-ray data: which was used as additional information for positioning Met residues only.

All ER-RAL complex crystal forms were suitable for flash-cooling by using a stream of N_2 at 100 K and 120 K. In all cases, the cryoprotectant consisted of mother liquor (well buffer composition) and 25% v/v MPD.

Owing to the sensitivity of the ER-R crystals all heavy atoms soaks were done in the exact mother liquor (taken from the well buffer) and the heavy atoms compounds were

always dissolved as a solid substance in these solutions. PCMBS-1 and KAuCN soaks were done for three days, PCMBS-2 for three weeks. All soaks done at 18°C. The cryo-solutions contained the heavy atom compounds at soaking concentration as well.

Pure ER-LBD is particularly refractive to crystallisation and suitable crystals were obtained after carboxymethylation of the three thiol groups.

EXAMPLE 3

Structure Determination of the Estrogen Receptor \alpha-Ligand Binding Domain

Crystals of the ER "-LBD complexed with either estradiol or raloxifen will diffract to medium resolution, are monoclinic and contain either a single dimer in the case of raloxifen or three dimers in the case of estrogen in the asymmetric unit (see Table 1). Multiple isomorphous replacement was used to determine the crystal structure of the ER-LBD-RAL complex. An initial multiple isomorphous replacement/density modified electron density map showed the position of the non-crystallographic two-fold rotation axis and allowed an initial polyalanine trace to be built on the resultant two-fold averaged map. Subsequent averaging between three different crystal forms of the RAL complex enabled corrections to be made to the initial trace. The remainder of the protein as yet not being unambiguously traced and most of the amino acid sequence to be assigned. The resultant model had an R value of 43%. Cycles of maximum likelihood refinement and manual rebuilding yielded a final model with acceptable R values and geometric parameters. The initial phase estimates were obtained for the estradiol (E2) complex by molecular replacement using the ER-LBD RAL dimer as a search model. Rotation in translation functions yielded the correct solution. Six-fold averaging between the three dimers in the crystal line asymmetric unit allowed both the missing parts of the structure to be traced and the positioning of E2 in the binding cavity to be determined. The structure was refined using both tight non-crystallographic restraints as well as average phase information to yield a final model with an Rcryst of 22.0 and R3 of 25.3 for all data between 20 and 3.1 ® (Table 1).

Results

The crystals produced in Example I and II were subjected to X-ray crystallographic studies which revealed that the LBD is folded into a characteristic "wedge-shaped" globular unit. It has a three-layered, anti-parallel \alpha-helical sandwich motif and is constructed from 8 major helices The motif comprises a central core layer of 3 helices (H5/6, H9 and H10) sandwiched between two additional layers of helices (H2-3 and H7, H8, H11). The arrangement of structural elements in this fashion creates a "molecular scaffold" maintaining a sizable ligand binding cavity at the "toe end" of the wedge-shaped domain. The remaining secondary structural elements, a small two stranded anti-parallel β-sheet (S1 and S2) and helix H12, are located at the "ligand binding end" of the molecule and flank the main three-layered motif (see Figure 2). From the N-terminus, the chain follows one turn of the distorted "-helix (H1), turns 90° and enters a short helix (H2) that lies parallel to the longest axis of the LBD. After helix H2, the chain continues in the same direction in an irregular extended conformation before tucking under the bottom of the molecule. At this stage, the chain turns back on itself through the long, bent, helix (H3). N-terminal portion of this helix forms part of the ligand binding cavity. The sequence has a proline at position 365 which is invariable and it is at this residue that the main chain takes a sharp (90°) change in direction, passes through a 310 helix (H4) before forming the first of three central helices (H5/6). Helix H5/6 can be geometrically described as a single unit, although it is kinked by 40° at the alanine residue at position 382 in a manner such that its C-terminal end is correctly positioned to form part of the E2 binding cavity. This helix is kinked and is distinguishing and is maintained by a series of hydrophobic interactions between leucines at 378 and 379 (H5) with a phenol at 367 and leucine at 453 all of which are highly conserved and are part of the nuclear receptor LBD signature motif (Wurst). From this position the sequence passes through a small \$ \ hairpin (S1/S2) covering one side of the binding cavity, and emerges on the other side of the molecule via the 3₁₀ helix H7. Helix H8 runs three quarters of the way up the long axis of the LBD, passes through a second central helix (H9) before turning back via a disordered loop to form a final helix H10.

At the end of H10, the polypeptide backbone changes direction and runs the full length of the ligand binding domain, in an anti-parallel direction to H8 in the form of helix 11. After a short turn the chain emerges on the opposite side to the S1/S2 β hairpin at helix H12, the core amphipathic helix of the AF-2 region.

DIMERISATION

Crystallographic studies also reveal that the receptor is dimerised. ER is sequestered in an inactive complex with heat shock protein 90 (hsp90) and other accessory factors in the absence of E2. Ligand binding initiates the disassembly of this complex and results in receptor dimerisation via domain E. The ligand-bound form of ER exists as a tight homodimer in solution and ER-LBDs are arranged as non-crystallographic dimers within both the E2 and RAL complex crystals. This quaternary arrangement almost certainly reflects the physiological state of ER-LBD in vivo as all crystal forms of the liganded ER-LBD obtained to date contained non-crystallographic dimers. The dimer axis coincides with the longest axis of the LBD with each molecule tilted approximately 15° away from the two position fold. This symmetric arrangement generates a molecule with dimensions of approximately 55Å high by 50Å wide by 35-60Å breadth. The observed quaternary arrangement locates the N and C termini of each monomer on the opposite "faces" of the dimer. The C terminus of each monomer projects towards the dimer axis while the N termini are far removed from the interface. The dimerisation surface is fairly extensive and encompasses about 15% (1,703 Å²) of each monomer's accessible surface area. The LBD's are positioned so that the H8/H11 face of each monomer lines up to form an additional, intermolecular helical layer. Contacts between the two molecules are made primarily through the H11 helices, which intertwine to form a rigid backbone, but also involve H8 from one monomer and H9 and H10 from the neighbouring monomer. The H11 helices are arranged as a bifurcated coiled coil with the side chains of the residues Leu 504, Ala 505, Leu 508, Leu 509 and Leu 511 which are interdigitated to form a partial "leucine zipper" motif at the coils end terminal N. This hydrophobic patch is flanked on either side by a network of hydrogen bonding residues. Arg 545 and Asn 519 make direct hydrogen bonds with Ser 512 and His 516 respectively. This overall monomer-monomer arrangement is unaffected by the nature of the ligand and seems to be maintained within the receptor super family. The observed ER-LBD dimer is identical in terms of gross monomer orientation and make up of the dimer interface to that of the crystallographic unliganded RXR- α homodimer (58% hydrophobic/42% hydrophillic).

The invariable nature of the LBD's quaternary structure therefore suggests that it provides a stable entity that facilitates separation of the two DNA binding domains in such a way as to allow optimal binding to EREs.

Such an elucidation of the 3-dimensional structure of the estrogen receptor ligand binding domain provides a useful tool for designing ligands for binding to the estrogen receptor. Such a detailed knowledge of the structure of the receptor enables prediction with accuracy whether a ligand binding to the receptor will act as an antagonist, a partial antagonist, an agonist or a partial agonist since the ligand-induced conformational changes can be anticipated.

EXAMPLE 4

Partial Homology Model of ERB

The coordinates obtained in Example I (ERα complexed with either estadiol or with raloxifine) were used to create two partial homology models of ERβ (complexed with estradiol and raloxifene respectively). This was accomplished by importing the ERα coordinates into version 6.4 of Sybyl (available from Tripos Associates, St. Louis, MO, U.S.A.). The "change" command in the Sybyl biopolymer module was used to mutate amino acids which differ between ERα and ERβ and which are in the vicinity of the ligand binding pocket. Four such residues were mutated: 1326V (Ile-326 to Val), L384M (Leu-384 to Met), M421I (Met-421 to Ile), F445Y (Phe-445 to Tyr). These partial ERβ homology models in conjunction with the experimental ERα coordinates were used to design isoform selective ligands as described in Example 5-51.

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Design of Ligands

Examples of ligands designed to fit the receptor have been produced as follows:

Example 5

2-(2,6-dimethylphenyl)-6-hydroxybenzo[β]thiophene (1).

- (a) To a solution of 6-methoxybenzo[β]thiophene (Graham et al, J. Med. Chem., 1989, 32, 2548.) (6 g, 36.5 mmol) in 50 ml of anhydrous tetrahydrofuran at -60°C was added n-butyllithium (20.5 ml, 41 mmol, 2.0 M solution in cyclohexane), dropwise via a dropping funnel. After stirring for 30 minutes, trimethyltin chloride (41 ml, 41 mmol, 1.0 M solution in hexanes) was introduced dropwise through a dropping funnel. The resulting mixture was allowed to warm to 0°C, stirred for 1 hour and then quenched with 100 ml of 1 M hydrochloric acid. The aqueous phase was extracted with ethyl acetate. The combined organic phases were dried over sodium sulphate and then concentrated in vacuo. This produced 9.24 g (28 mmol, 77%) of 2-trimethylstannyl-6-methoxybenzo[β]thiophene as white semicrystals. ¹H NMR (CDCl₃) 7.66 (d, J = 8.6 Hz, 1H), 7.34 (d, J = 2.2 Hz, 1H), 7.29 (s, 1H), 6.95 (dd, J = 8.6 Hz, 2.2 Hz, 1H), 3.86 (s, 3H), 0.39 (s, 9H).
- (b) A mixture of 370 mg (2 mmol) 2-bromo-m-xylene, 115 mg (0.1 mmol) tetrakis triphenylphosphinepalladium (0) and 160 mg (2 mmol) of cupric oxide in 8 ml of N,N-dimethylformamide was stirred at 100°C under nitrogen. After 5 minutes, 981 mg (3 mmol) of 2-trimethylstannyl-6-methoxybenzo[β]thiophene (example 1a) in 2 ml of N,N-dimethylformamide was added all at once to the reaction mixture. The reaction was heated for 2 hours and then allowed to reach room temperature. The resulting mixture was concentrated, dissolved in ethylacetate, filtered through a pad of silica and concentrated. The crude product was purified on a chromatotron (silica, 99:1, petroleum ether/ethyl acetate) producing 328 mg (1.22 mmol, 61%) of 2-(2,6-dimethylphenyl)-6-methoxybenzo[β]thiophene a yellowish crystals. H NMR (CDCl₃) 7.89 (d, J = 8.7 Hz, 1H), 7.32-7.59 (m, 4H), 7.23 (dd, J = 8.7 Hz, 2.2 Hz, 1H), 7.18 (s, 1H), 4.12 (s, 3H), 2.46 (s, 6H).

(c) 145 mg (0.54 mmol) of 2-(2,6-dimethylphenyl)-6-methoxybenzo[β]thiophene (example 1b) was dissolved in 15 ml of dichloromethane, to the stirred solution was added boron trifluoride dimethylsulfide complex (1.5 ml). The solution was stirred at room temperature under nitrogen in the dark for 15 hours. The reaction mixture was quenched with 10 ml of water, extracted with dichloromethane, dried over magnesium sulphate and concentrated. The crude product was purified on a chromatotron (silica, 80:20, petroleum ether/ ethyl acetate) producing 94.1 mg (0.37 mmol, 69%) of 2-(2,6-dimethylphenyl)-6-hydroxybenzo[β]thiophene as white crystals. MP 95-96°C. ¹H NMR (CDCl₃) 7.63 (d, J = 8.6, 1H), 7.08-7.31 (m, 4H), 6.92 (s, 1H), 6.91 (dd, J = 8.6, 2.2 Hz, 1H), 4.91 (s, 1H), 2.20 (s, 6H).

Example 6

2-(2-ethyl-6-methylphenyl)-6-hydroxybenzo[β]thiophene (2).

- (a) The cross-coupling of 492 mg (2 mmol) 2-ethyl-6-methyliodobenzene, with 981 mg (3 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude product was purified on a chromatotron (silica, 99:1, petroleum ether/ ethyl acetate) producing 438 mg (1.55 mmol, 78%) of 2-(2-ethyl-6-methylphenyl)-6-methoxybenzo[β]thiophene as a colourless oil. H NMR (CDCl₃) 7.67 (d, J = 8.9 Hz, 1H), 7.08-7.36 (m, 4H), 7.01 (dd, J = 8.9 Hz, 2.2 Hz 1H), 6.96 (s, 1H), 3.89 (s, 3H), 2.54 (q, J = 7.6 Hz, 2H), 2.19 (s, 3H), 1.12 (t, J = 7.6 Hz, 3H).
- deprotection 100 (b) o f m g (0.35)mmol) o f 2-(2-ethyl-6-methylphenyl)-6-methoxybenzo[\(\beta\)]thiophene (example 2(a)) was accomplished by the procedure set forth in example 1(c). The crude product was purified on a chromatotron (silica, 90:10, petroleum ether/ ethyl acetate) producing 69 mg (0.26 mmol, 73%) of 2-(2-ethyl-6-methylphenyl)-6-hydroxybenzo[β]thiophene as white semicrystals. ¹H NMR (CD₃OD) 7.59 (d, J = 8.7, 1H), 7.06-7.25 (m, 4H), 6.90 (s, 1H), 6.88 (dd, J = 8.7, 2.2 Hz, 1H), 2.51 (q, J = 7.6 Hz, 2H), 2.15 (s, 3H), 1.09

(t, J = 7.6 Hz, 3H).

Example 7

2-(2.6-dimethyl-4-hydroxyphenyl)-6-hydroxybenzo[β]thiophene (3).

- (a) The cross-coupling of 402 mg (2 mmol) 4-bromo-3,5-dimethylphenol, with 981 mg (3 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude product was purified on a chromatotron (silica, 90:10, petroleum ether/ ethyl acetate) producing 210 mg (0.74 mmol, 37%) of 2-(2,6-dimethyl-4-hydroxyphenyl)-6-methoxybenzo[β]thiophene as yellow crystals. HNMR (CDCl₃) 7.88 (d, J = 8.7 Hz, 1H), 7.55 (d, J = 2.5 Hz, 1H), 7.22 (dd, J = 8.7 Hz, 2.5 Hz 1H), 7.14 (s. 1H), 6.83 (s, 2H), 4.94 (s, 1H), 4.11 (s, 3H), 2.38 (s. 6H).
- (b) The deprotection of 100 mg (0.35 mmol) of 2-(2.6-dimethyl-4-hydroxyphenyl)-6-methoxybenzo[β]thiophene (example 3(a)) was accomplished by the procedure set forth in example 1(c). The crude product was purified on a chromatotron (silica, 80:20, petroleum ether/ethyl acetate) producing 52 mg (0.19 mmol, 54%) of 2-(2,6-dimethyl-4-hydroxyphenyl) -6-hydroxybenzo[β]thiophene as white crystals. MP 202-204°C, ¹H NMR (CD₃OD) 7.56 (d, J = 8.7, 1H), 7.19 (d, J = 2.2 Hz, 1H), 6.86 (dd, J = 8.7, 2.2 Hz, 1H), 6.84 (s, 1H), 6.54 (s, 2H), 2.10 (s, 6H).

Example 8

2-(2-methylphenyl)-6-hydroxybenzo[β]thiophene (4).

(a) The cross-coupling of 340 mg (2 mmol) 2-bromotoluene, with 981 mg (3 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b) The crude product was purified on a chromatotron (silica, 99:1, petroleum ether/ethyl acetate) producing 500 mg (1.97 mmol, 98%) of

2-(2-methylphenyl)-6-methoxybenzo[β]thiophene as white crystals. ¹H NMR (CDCl₃) 7.66 (d, J = 8.7 Hz, 1H), 7.19-7.49 (m, 5H), 7.15 (s, 1H), 6.99 (dd, J = 8.7, 2.3 Hz, 1H), 3.88 (s, 3H), 2.48 (s, 3H).

(b) The deprotection of 125 mg (0.49 mmol) of 2-(2-methylphenyl) -6-methoxybenzo[β]thiophene (example 4(a)) was accomplished by the procedure set forth in example 1(c). The crude product was purified on a chromatotron (silica, 90:10, petroleum ether/ ethyl acetate) producing 60 mg (0.23 mmol, 47%) of 2-(2-methylphenyl)-6-hydroxybenzo[β]thiophene as white crystals. MP 97-98°C, ¹H NMR (CDCl₃) 7.63 (d, J = 8.4 Hz, 1H), 7.18-7.48 (m, 5H), 7.14 (s, 1H), 6.91 (dd, J = 8.4, 2.3 Hz, 1H), 4.86 (s, 1H), 1.56 (s, 3H).

Example 9

 $2-(2-chloro-6-methylphenyl)-6-hydroxybenzo[\beta]thiophene (5).$

- (a) The cross-coupling of 505 mg (2 mmol) 3-chloro-2-iodotoluene, with 981 mg (3 mmol) of product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude product was purified on a chromatotron (silica, 99:1, petroleum ether/ethyl acetate) producing 439 mg (1.52 mmol, 76%) of 2-(2-chloro-6-methylphenyl) -6-methoxybenzo[β]thiophene as a yellow oil. ¹H NMR (CDCl₃) 7.68 (d, J = 8.7 Hz, 1H), 7.15-7.36 (m, 4H), 7.03 (s, 1H), 7.01 (dd, J = 8.7, 2.2 Hz, 1H), 3.88 (s, 3H), 2.25 (s, 3H).
- (b) The deprotection of 100 mg (0.35 mmol of 2-(2-chloro-6-methylphenyl) -6-methoxybenzo[β]thiophene (example 5(a)) was accomplished by the procedure set forth in example 1(c). The crude product was purified on a chromatotron (silica, 90:10, petroleum ether/ ethyl acetate) producing 44 mg (0.16 mmol, 46%) of -2-(2-chloro-6-methylphenyl)-6-hydroxybenzo[β]thiophene as a yellowish oil. ¹H NMR (CD₃OD) 7.62 (d, J = 8.7 Hz, 1H), 7.18-7.35 (m, 4H), 6.99 (s, 1H), 6.89 (dd, J = 8.7, 2.2 Hz, 1H), 2.23 (s, 3H).

Example 10

2-(2-methylnaphth-1-yl)-6-hydroxybenzo[β]thiophene (6).

- (a) The cross-coupling of 221 mg (1 mmol) 1-bromo-2-methylnaphthalene, with 491 mg (1.5 mmol) of product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude product was purified on a chromatotron (silica, 99:1, petroleum ether/ ethyl acetate) producing 159 mg (0.52 mmol, 52%) of 2-(2-methylnaphth-1-yl)-6-methoxybenzo[β]thiophene as white crystals. ¹H NMR (CDCl₃) 7.66-7.88 (m, 4H), 7.30-7.48 (m, 4H), 7.11 (s, 1H), 7.04 (dd, J = 8.7, 2.2 Hz, 1H), 3.91 (s, 3H), 2.40 (s, 3H).
- (b) The deprotection of 110 mg (0.36 mmol) of 2-(2-methylnaphth-1-yl) -6-methoxybenzo[β]thiophene (example (6a)) was accomplished b the procedure set forth in example 1(c). The crude product was purified on a chromatotron (silica, 90:10. petroleum ether/ethyl acetate) producing 52 mg (0.18 mmol, 50%) of -2-(2-methylnaphth-1-yl)-6-hydroxybenzo[β]thiophene as white semi crystals. ¹H NMR (CD₃COCD₃) 8.60 (s, 1H) 7.87-8.05 (m, 2H), 7.74 (d, J = 8.7 Hz, 1H), 7.65-7.71 (m, 1H), 7.38-7.54 (m, 4H) 7.18 (s, 1H), 7.02 (dd, J = 8.7, 2.2 Hz, 1H), 2.39 (s, 3H).

Example 11

2-(2,5-dimethyl-4-hydroxyphenyl)-6-hydroxybenzo[β]thiophene (7).

(a) The cross-coupling of 248 mg (1 mmol) 2,5-dimethyl-4-iodophenol, with 491 mg (1.5 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude product was purified on a chromatotron (silica, 9:1, petroleum ether/ ethyl acetate) producing 130 mg (0.46 mmol, 46%) of 2-(2,5-dimethyl-4-hydroxyphenyl)-6-methoxybenzo[β]thiophene as white crystals. ¹H NMR (CDCl₃) 8.34 (s, 1H), 7.69 (d, J = 8.8 Hz, 1H), 7.45 (d, J = 2.3 Hz, 1H), 7.19 (s, 1H), 7.17 (s, 1H), 6.98 (dd, J = 8.8, 2.3 Hz, 1H), 6.78 (s, 1H), 3.87 (s, 3H), 2.34

(s, 3H), 2.20 (s, 3H).

(b) The deprotection of 35 mg (0.12 mmol) of 2-(2,5-dimethyl -4-hydroxyphenyl)-6-methoxybenzo[β]thiophene (example (6a)) was accomplished by the procedure set forth in example 1(c). The crude product was purified on a chromatotron (silica, 70:30, petroleum ether/ ethyl acetate) producing 26 mg (0.096 mmol, 80%) of 2-(2,5-dimethyl-4-hydroxyphenyl)-6-hydroxybenzo[β]thiophene as white crystals. MP 134-136°C, ¹H NMR (CD₃COCD₃) 8.41 (s broad, 2H) 7.63 (d, J = 8.7 Hz, 1H), 7.30 (d, J = 2.2 Hz, 1H), 7.18 (s, 1H), 7.13 (s, 1H) 6.93 (dd, J = 8.7, 2.2 Hz, 1H), 6.77 (s,1H), 2.34 (s, 3H), 2.19 (s, 3H).

Example 12

2-(4-hydroxyphenyl)-6-hydroxybenzo[β]thiophene (8).

Prepared according to (Hauser et al, WO 96/30361).

Example 13

2-(2-benzylphenyl)-6-hydroxybenzo[β]thiophene (9).

The cross-coupling of 124 mg (0.5 mmol) 2-bromodiphenylmethane, with 246 mg (0.75 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude product was deprotected by the procedure set forth in example 1 (c). It was purified on a chromatotron (silica, 92:8, petroleum ether/ ethyl acetate) producing 108 mg (0.34 mmol, 68%) 2-(2-benzylphenyl) -6-hydroxybenzo[β]thiophene as slightly pink crystals. ¹H NMR (CD₃COCD₃) 8.55 (s 1H) 7.62 (d, J = 8.4 Hz, 1H), 7.04-7.51 (m, 11H), 6.93 (dd, J = 8.5, 2.5 Hz, 1H), 4.19 (s, 2H).

Example 14

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Example 14

$2-(4-hydroxynapht-1-yl)-6-hydroxy[\beta]thiophene (10)$

The cross-coupling of 119 mg (0.5 mmol) 1-bromo-4-methoxynaphthalene, with 246 mg (0.75 mmol) of the product from $\mathbf{1}(a)$ was accomplished by the procedure set forth in example $\mathbf{1}(b)$. The crude product was deprotected by the procedure set forth in example 1 (c). It was purified on a chromatotron (silica, 8:2, petroleum ether/ ethyl acetate) producing 9 mg (0.03 mmol, 6.2%) 2-(4-hydroxynapht-1-yl)-6-hydroxy[β]thiophene(10) as dark brown crystals. H NMR (CD₃COCD₃) 9.34 (s, 1H), 8.55 (s 1H), 8.31-8.38 (m, 1H), 8.20-8.27 (m, 1H), 7.72 (d, J = 8.4 Hz, 1H), 7.48-7.58 (m, 2H), 7.48 (d, J = 7.7, 1H), 7.37 (d, J = 2.2, 1H), 7.34 (s, 1H), 7.00 (d, J = 7.7, 1H), 6.98 (dd, J = 8.4, 2.2 Hz, 1H).

Example 15

2-(2-methyl-3-chlorophenyl)-6-hydroxybenzo[β]thiophene (11).

The cross-coupling of 126 mg (0.5 mmol) 2-chloro-6-iodotoluene, with 246 mg (0.75 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude product was deprotected by the procedure set forth in example 1 (c). It was then purified on a chromatotron (silica, 92:8, petroleum ether/ethyl acetate) producing 88 mg (0.32 mmol, 64.1%) of 2-(2-methyl-3-chlorophenyl)-6-hydroxybenzo[β]thiophene (11). HNMR (CDCl₃) 7.72 (d, J = 8.7 Hz, 1H), 7.29-7.41 (m, 2H), 7.27 (d, J = 2.5, 1H), 7.17 (d, J = 7.91, 1H), 7.10 (s, 1H), 6.92 (dd, J = 8.7, 2.5 Hz, 1H), 2.46 (s, 3H).

Example 16

2-(2-methyl-5-chlorophenyl)-6-hydroxybenzo[β]thiophene (12).

The cross-coupling of 126 mg (0.5 mmol) 4-chloro-2-iodotoluene, with 246 mg (0.75 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude product was deprotected by the procedure set forth in example 1 (c). It was then purified on a chromatotron (silica, 92:8, petroleum ether/ethyl acetate) producing 88 mg (0.32 mmol, 64.1%) of 2-(2-methyl-5-chlorophenyl) -6-hydroxybenzo[β]thiophene (12). H NMR (CDCl₃) 7.63 (d, J = 8.7 Hz, 1H), 7.43 (d, J = 2.0 Hz, 1H), 7.27 (d, J = 2.2, 1H), 7.19-7.23 (m, 2H), 7.14 (s, 1H), 6.92 (dd, J = 8.5, 2.2 Hz, 1H), 2.41 (s, 3H).

Example 17

2-(2-methyl-4-chlorophenyl)-6-hydroxybenzo[β]thiophene (13).

The cross-coupling of 103 mg (0.5 mmol) 2-bromo-5-chlorotoluene, with 246 mg (0.75 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude product was deprotected by the procedure set forth in example 1 (c). It was then purified on a chromatotron (silica, 92:8, petroleum ether/ethyl acetate) producing 118 mg (0.43 mmol, 85.9%) 2-(2-methyl-4-chlorophenyl) -6-hydroxybenzo[β]thiophene (13) as slightly pink crystals. ¹H NMR (CD₃COCD₃) 8.63 (s. 1H), 7.69 (d, J = 8.7 Hz, 1H), 7.45 (d, J = 8.4 Hz, 1H), 7.26-7.41 (m, 4H). 6.92 (dd, J = 8.4, 2.2 Hz, 1H), 2.47 (s, 3H).

Example 18

2-(2.5-hydroxy-4-bromophenyl)-6-hydroxybenzo[β]thiophene (14).

The cross-coupling of 222 mg (0.75 mmol) 1,4-dibromo-2,5-dimethoxybenzene with 367 mg (1.125 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b). It was then purified on a chromatotron (silica, 95:5, petroleum ether/ acetone) producing 65.5 mg (0.17 mmol, 23%) of 2-(2.5-methoxy-4-bromophenyl)-6-methoxybenzo[\beta]thiophene. 25 mg (0.066 mmol)

14.1 mg (0.042 mmol. 63.4%) of 2-(2,5-hydroxy-4-bromophenyl) -6-hydroxybenzo[β]thiophene. H NMR (CD₃COCD₃) 8.84 (s, 1H), 8.54 (s, 1H), 8.33 (d, J = 8.74 Hz, 1H), 7.81 (s, 1H), 7.69 (d, J= 8.4 Hz, 1H), 7.34 (d, J = 2.2 Hz, 1H), 7.28 (s, 1H), 7.14 (s, 1H), 6.92 (dd, J = 8.4, 2.2 Hz, 1H).

Example 19

2-(2-methyl-4-nitrophenyl)-6-hydroxybenzo[β]thiophene (15).

- (a) The cross-coupling of 432 mg (2.0 mmol) 2-bromo-5- nitrotoluene with 982 mg (3.0 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude product was purified on a chromatotron (silica, 8:2, petroleum ether/ ethyl acetate) producing 681 mg (about 75% pure) of 2-(2-methyl-4-nitrophenyl)-6-methoxybenzo[β]thiophene.
- 2-(2-methyl-4deprotection of 100 mg (0.33)mmol) (b) The nitrophenyl)-6-methoxybenzo[β]thiophene (example (15a)) was accomplished by the procedure set forth in example 1(c). The crude product was purified on a chromatotron (silica, 70:30, petroleum ether/ ethyl acetate) producing 73 mg (0.26 mmol, 78%) of 2-(2-methyl-4-nitrophenyl)-6-hydroxybenzo[β]thiophene. H NMR (CDCl₃) 8.16 (d broad, J = 2.1 Hz, 1H) 8.08 (dd, J = 8.5, 2.1 Hz, 1H), 7.68 (d, J = 8.5 Hz, 1H), 7.60 (d, J = 8.5, 1H), 7.29 (d, J = 2.4 Hz, 1H) 7.27 (s, 1H), 6.94 (dd, J = 8.5, 2.4 Hz, 1H),5.15 (s, 1H), 2.59 (s, 3H).

Example 20

2-(2-methyl-4-aminophenyl)-6-hydroxybenzo[β]thiophene (16).

50 mg (0.18 mmol) of 2-(2-methyl-4-nitrophenyl) -6-hydroxybenzo[β]thiophene (example (15(b)) was dissolved in 5 ml of ethanol and 198 mg (0.88 mmol) of tin dichloride dihydrate was added. The mixture was heated to 70°C under a nitrogen

atmosphere for 3 hours. Hydrochloric acid (1 M) was added and then the aqueous phase was extracted with ethyl acetate. The combined organic phases were washed with brine, dried over magnesium sulphate and then concentrated in vacuo. The crude product was purified on a chromatotron (silica, 6:4, petroleum ether/ ethyl acetate) producing 22 mg (0.086 mmol, 48%) of 2-(2-methyl-4-aminophenyl)-6-hydroxybenzo[β]thiophene. H NMR (CD₃OD) 7.54 (d, J = 8.6, 1H), 7.18 (d, J = 2.4 Hz, 1H), 7.17 (d, J = 8.6, 1H), 7.00 (s, 1H), 6.84 (dd, J = 8.6, 2.4 Hz, 1H), 6.64 (d, J = 2.4 Hz, 1H), 6.58 (dd, J = 8.6, 2.4 Hz), 2.37 (s, 3H).

Example 21

2-(2-methyl-3-nitrophenyl)-6-hydroxybenzo[β]thiophene (17).

- (a) The cross-coupling of 432 mg (2.0 mmol) 2-bromo-6- nitrotoluene with 982 mg (3.0 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude product was purified on a chromatotron (silica, 95:5, petroleum ether/ ethyl acetate) producing 114 mg (0.38 mmol, 13%) of 2-(2-methyl-3-nitrophenyl)-6-methoxybenzo[β]thiophene.
- 2-(2-methyl-3deprotection of 200 mg (0.67)mmol) The (b) nitrophenyl)-6-methoxybenzo[β]thiophene (example (17a)) was accomplished by the procedure set forth in example 1(c). The crude product was purified on a chromatotron (silica, 70:30, petroleum ether/ ethyl acetate) producing 101 mg (0.35 mmol, 53%) of 2-(2-methyl-3-nitrophenyl)-6-hydroxybenzo[β]thiophene. H NMR (CDCOCD₃) 8.67 (s, 1H), 7.86 (dd, J = 8.0, 1.2 Hz, 1H), 7.76 (dd, J = 7.7, 1.2 Hz, 1H), 7.73 (d, J = 8.7Hz, 1H), 7.54 (m, 1H), 7.38 (d, J = 2.1 Hz, 1H), 7.36 (s, 1H), 7.00 (dd, J = 8.7, 2,1 Hz, 1H), 5.15 (s, 1H), 2.52 (s, 3H).

Example 22

2-(2-methyl-3-aminophenyl)-6-hydroxybenzo[β]thiophene (18).

350 mg (1.23 mmol) of 2-(2-methyl-3-nitrophenyl) -6-hydroxybenzo[β]thiophene

(example (17(b)) was dissolved in 10 ml of ethanol and 1384 mg (6.1 mmol) of tin dichloride dihydrate was added. The mixture was heated to 70°C under a nitrogen atmosphere for 3 hours. Hydrochloric acid (1 M) was added and then the aqueous phase was extracted with ethyl acetate. The combined organic phases were washed with brine, dried over magnesium sulphate and then concentrated in vacuo. The crude product was purified on HPLC (reversed phase, C18, gradient acetonitrile/ water + 0.05 trifluoroacetic acid) producing 27 mg (0.10 mmol, 8.1%) of 2-(2-methyl-3-aminophenyl)-6-hydroxybenzo[β]thiophene. ¹H NMR (CD₃OD) 8.93 (s, 1H broad), 7.65 (d, J = 8.8, 1H), 7.33 (d, J = 2.5 Hz, 1H), 7.12 (s, 1H), 6.92-7.00 (m, 2H), 6.71-6.78 (m, 2H), 4.69 (s, 2H broad), 2.20 (s, 3H).

Example 23

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 $2-(2-methyl-3-bromo-5-hydroxyphenyl)-6-hydroxybenzo[<math>\beta$]thiophene (19).

- (a) The cross-coupling of 369 mg (1.3 mmol) 2,6-dibromo-4- methoxytoluene with 636 mg (1.95 mmol) of the product from $\mathbf{1}(a)$ was accomplished by the procedure set forth in example $\mathbf{1}(b)$. The crude product was purified on a chromatotron (silica. 98:2, petroleum ether/ ethyl acetate) producing 220 mg (0.61 mmol, 46.6%) of 2-(2-methyl-3-bromo-5-methoxyphenyl)-6-methoxybenzo[β]thiophene.
- mmol) 2-(2-methyl-3-bromo-5mg (0.19)deprotection of 70 (b) The methoxyphenyl)-6-methoxybenzo[β]thiophene (example (19a)) was accomplished by the procedure set forth in example 1(c). The crude product was purified on a chromatotron (silica. 8:2, petroleum ether/ ethyl acetate) producing 55 mg (0.16 mmol, 86%) of 2-(2-methyl-3-bromo-5- hydroxyphenyl)-6-hydroxybenzo[β]thiophene. 'H NMR (CDCOCD₃) 8.66 (s, 1H), 7.69 (d, J = 8.4, 1H), 7.34 (d, J = 2.2 Hz, 1H), 7.23 (s, 1H), 7.15 (d, J = 2.5 Hz, 1H), 6.99 (d, J = 2.2 Hz, 1H), 7.00 (dd, J = 8.4, 2,2 Hz, 1H), 6.94 (d, J = 2.5 Hz, 1H), 2.38 (s, 3H).

Example 24

2-(2-methyl-5-hydroxyphenyl)-6-hydroxybenzo[β]thiophene (20).

- a) 30 mg (0.08)mmol) 2-(2-methyl-3-bromo-5-methoxyphenyl) -6-methoxybenzo[β]thiophene (example (19a) was dissolved in 2 ml of tetrahydrofuran. The mixture was cooled to -70°C and butyllithium (0.12 mmol) was added to the reaction mixture. The reaction mixture was stirred for 2.5 hours at -70°C and then at room temperature overnight. The reaction mixture was quenched with aqueous ammonium chloride, extracted with ethyl acetate and dried over magnesium sulphate. This produced 30 mg of crude 2-(2-methyl-5-methoxyphenyl) -6-methoxybenzo[β]thiophene.
- The b) deprotection of 30 mg (0.10)mmol) 2-(2-methyl-5methoxyphenyl)-6-methoxybenzo[β]thiophene (example (20a)) was accomplished by the procedure set forth in example 1(c). The crude product was purified on HPLC (reversed phase, C18, gradient, acetonitrile/water + 0.05 trifluoroacetic acid) producing 6.7 (0.026)mmol, 24%) of 2-(2-methyl-5-hydroxyphenyl) -6-hydroxybenzo[β]thiophene. ¹H NMR (CD₃COCD₃) 8.55 (s, 1H), 8.29 (s, 1H), 7.67 (dd, J = 8.5, 2.2 Hz, 1H), 7.33 (t, 1H), 7.24 (d, J = 2.5, 1H), 7.13 (dd, J = 8.2, 2.0 Hz,1H), 6.92-6.99 (m, 2H), 6.76 (dt, 1H), 2.35 (d, J = 2.2 Hz, 3H).

Example 25

2-phenyl-6-hydroxybenzo[β]thiophene (21).

The cross-coupling of 157 mg (1.0 mmol) bromobenzene with 491 mg (1.5 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude product was deprotected by the procedure set forth in example 1 (c). It was purified on a chromatotron (silica, 9:1, petroleum ether/ ethyl acetate) producing 81 mg (0.36 mmol, 36%) 2-phenyl-6-hydroxybenzo[β]thiophene. ¹H NMR (CD₃COCD₃) 8.65 (s 1H), 7.60-7.75 (m, 4H), 7.28-7.48 (m, 4H), 6.95 (dd, J = 8.5, 2.5 Hz, 1H).

Example 26

2-(4-hydroxyphenyl)-benzo[β]thiophene (22).

- (a) The stannylation of 3 g (22.4 mmol) of benzo[β]thiophene was accomplished by the procedure set forth in example 1(a). This produced 6.3 g (21.3 mmol) of 2-trimethylstannylbenzo[β]thiophene.
- (b) The cross-coupling of 468 mg (2.0 mmol) 4-iodophenol with 889 mg (3.0 mmol) of the product from 22(a) was accomplished by the procedure set forth in example 1(b). The crude product was deprotected by the procedure set forth in example 1 (c) and then purified on a chromatotron (silica, 9:1, petroleum ether/ ethyl acetate) and recrystalised (petroleum ether/ ethyl acetate) producing 20 mg (0.09 mmol, 4%) of 2-(4-hydroxyphenyl)-benzo[β]thiophene. ¹H NMR (CD₃COCD₃) 8.70 (s 1H), 7.88 (m, 1H), 7.79 (m, 1H), 7.56-7.69 (m, 3H), 7.25-7.38 (m, 2H), 6.90-7.00 (m, 2H).

Example 27

 $2-(2-trifluoromethyl-6-fluorophenyl)-6-hydroxybenzo[<math>\beta$]thiophene (23).

Produced in a parallell solution phase way. A mixture of 61 mg (0.25 mmol) 2-bromo-3-fluorobenzotrifluoride, (0.013)mmol) tetrakis 15 mg triphenylphosphinepalladium (0) and 20 mg (0.25 mmol) of cupric oxide in 1 ml of N,N-dimethylformamide was stirred at 100°C under nitrogen. After 5 minutes, 123 mg (0.38 mmol) of 2-trimethylstannyl-6-methoxybenzo[β]thiophene (example 1(a)) in 2 ml of N,N-dimethylformamide was added all at once to the reaction mixture. The solution was heated to 100°C for 3 hours, concentrated on a speed-vac, dissolved in dichloromethane, filtered through a silica pad and then concentrated again. The product was dissolved in 1.5 ml of dichloromethane and 1 ml of boron trifluoride dimethylsulfide complex was added. The reaction mixture was stirred overnight in darkness, quenched with water and extracted with dichloromethane. The organic phase

was dried by passing it through sodium sulphate dryingtubes and then it was concentrated in a speed-vac. The crude product was purified on HPLC (silica, n-heptane + 0.5% acetic acid to ethyl acetate + 0.5% acetic acid as gradient eluent) producing 1.5 mg (0.005 mmol, 2%) of 2-(2-trifluoromethyl-6-fluorophenyl)-6-hydroxybenzo[β]thiophene. HNMR (CD₃COCD₃) 8.72 (s, 1H broad), 7.71-7.78 (m, 3H), 7.55-7.65 (m, 1H), 7.37 (d, J = 2.2. Hz, 1H), 7.29 (s, 1H), 6.99 (dd, J = 8.7, 2.2 Hz, 1H).

Example 28

6-(6-hydroxy-2-benzo[β]thienyl)-4,5-dimethylbenzo-2,1,3-thiadiazole (24).

The cross-coupling of 61 mg (0.25 mmol) 6-bromo-4,5-dimethylbenzo-2, 1,3-thiadiazole with 123 mg (0.38 mmol) of the product from 1(a) and the subsequent deprotection was accomplished by the procedure set forth in example 23. The crude product was purified on HPLC (silica, n-heptane + 0.5% acetic acid to ethyl acetate + 0.5% acetic acid as gradient eluent) producing 3.6 mg (0.012 mmol, 4.6%) of 6-(6-hydroxybenzo[β]thien-2-yl)-4,5-dimethylbenzo-2,1,3-thiadiazole. ¹H NMR (CD₃COCD₃) 7.92 (s 1H), 7.74 (d, J = 8.5, 1H), 7.38 (d, J = 2.2 Hz, 1H), 7.37 (s, 1H), 7.01 (dd, J = 8.5, 2.2 Hz, 1H), 2.76 (s, 3H), 2.50 (s, 3H).

Example 29

2-(4-methyl-3-thienyl)-6-hydroxybenzo[β]thiophene (25).

The cross-coupling of 44 mg (0.25 mmol) 3-bromo-4-methylthiophene with 123 mg (0.38 mmol) of the product from 1(a) and the subsequent deprotection was accomplished by the procedure set forth in example 23. The crude product was purified on HPLC (silica, n-heptane+ 0.5% acetic acid to ethyl acetate + 0.5% acetic acid as gradient eluent) producing 22 mg (0.09 mmol, 36%) 2-(4-methyl-3-thienyl)-6-hydroxybenzo[β]thiophene. ¹H NMR (CD₃COCD₃) 8.57 (s

1H), 7.66 (d, J = 8.4, 1H), 7.53 (d, J = 3.2 Hz, 1H), 7.35 (s, 1H), 7.32 (m, 1H),

Example 30

2-(3,4,5-trimethyl-2-thienyl)-6-hydroxybenzolβlthiophene (26).

The cross-coupling of 252 mg (01.0 mmol) 2-iodo-3,4,5-trimethylthiophene with 491 mg (1.5 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude 2-(3,4,5-trimethyl-2-thienyl)-6-methoxybenzo[β] thiophene was deprotected by the procedure set forth in example 1 (c) and then purified on a chromatotron (silica, 9:1, petroleum ether/ ethyl acetate) producing 180 mg (0.625 mmol, 63%) of 2-(3,4,5-trimethyl-2-thienyl)-6-hydroxybenzo[β] thiophene. ¹H NMR (CD₃COCD₃) 8.55 (s, 1H), 7.67 (d, J = 8.7 Hz, 1H), 7.32 (d, J = 2.2 Hz, 1H), 7.06 (d, J= 0.7 Hz, 1H), 6.95 (dd, J= 8.7, 2.2 Hz, 1H), 2.34 (s, 3H), 2.30 (s, 3H), 1.96 (s, 3H).

Example 31

2-(5-(1,3-dimethyluracilyl))-6-hydroxybenzo[β] thiophene (27).

- (a) The cross-coupling of 266 mg (1.0 mmol) 5-iodo-1,3-dimethyluracil with 491 mg (1.5 mmol) of the product from 1(a) was accomplished by the procedure set forth in example 1(b). The crude product was purified on a chromatotron (silica, 40:1, dichloromethane/ ethyl acetate) producing 211 mg (0.625 mmol, 63%) of 2-(5-(1,3-dimethyluracilyl))-6-methoxybenzo[β] thiophene.
- (b) The deprotection of 30 mg (0.10 mmol) of 2-(5-(1,3-dimethyluracilyl))-6-methoxybenzo[β] thiophene (example (27a)) was accomplished by the procedure set forth in example 1(c). The crude product was purified on a chromatothron (silica, 9:1, petroleum ether/ ethyl acetate) producing 1.2 mg (0.004 mmol, 4.2%) of

 $2-(5-(1.3-\text{dimethyluracilyl}))-6-\text{hydroxybenzo}[\beta]$ thiophene ¹ H NMR (CDCl₃) 7.74 (s, 1H), 7.61 (d, J = 8.7 Hz, 1H), 7.54 (s, 1H), 7.10-7.30 (m, 1H), 7.13 (dd, J = 8.7, 2.3 Hz, 1H), 3.87 (s, 3H), 3.51 (s, 3H).

Example 32

[2-(4-hydroxyphenyl)-6-hydroxybenzo[\beta] thien-3-yl][phenyl]methanone (28).

- (a) To 200 mg, (0.74 mmol) 6-methoxy-2-(4-methoxyphenyl)benzo[β] thiophene (Hauser et al, WO 96/30361) and 110 mg (0.78 mmol) benzoyl chloride in dichloro methane (5 ml) was added 740 mg (5.6 mmol) aluminium chloride. The reaction mixture was stirred for 5 hours at room temperature. The reaction was quenched by the addition of ethyl acetate and 1 M hydrochloric acid. The organic layer was separated and the aqueous phase was extracted with ethyl acetate. The combined organic phases were dried over magnesium sulphate, filtered and concentrated. The crude product was purified on a chromatotron (silica, 95:5, petroleum ether/ethyl 47%) 131 m g (0.35)mmol, acetate) producing [2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl]phenylmethanone as yellow crystals. 1 H NMR (CDCl₃) 7.72-7.80 (m, 2H) 7.59 (d, J = 8.9 Hz, 1H), 7.36-7.43 (m, 1H), 7.21-7.34 (m, 5H), 6.97 (dd, J = 8.9, 2.5 Hz, 2H) 6.72 (m, 1H), 3.88 (s, 3H), 3.72 (s, 3H).
- (b) 70 mg, (0.19 mmol) [2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl] phenylmethanone (example 28a) was dissolved in dichloromethane (5 ml), put under nitrogen atmosphere and cooled to -5°C. To the stirred solution was added 0.56 ml (0.56 mmol) 1M BBr₃ dropwise. The reaction mixture was stirred for 1 hour at 5°C, poured into ice water and extracted with ethyl acetate. The organic phase was dried over magnesium sulphate, filtered and concentrated. The crude product was purified on a chromatotron (silica, 75:25 to 50:50, petroleum ether/ ethyl acetate as gradient eluent) producing 46 mg (0.13 mmol, 71%) of [2-(4-hydroxyphenyl) -6-hydroxybenzo[β] thien-3-yl]phenylmethanone as yellow crystals. MP 214-217°C,

¹H nmr (CD₃COCD₃) 8.74 (s, 1H), 8.64 (s, 1H), 7.70-7.77 (m, 2H), 7.20-7.54 (m, 7H), 6.96 (dd, J = 8.7, 2.4 Hz, 1H), 6.68-6.76 (m, 2H).

Example 33

[2-(4-hydroxyphenyl)-6-hydroxybenzo[\beta] thien-3-yl][2-naphthyl]methanone (29).

- (a) The acylation of 150 mg, (0.55 mmol) 6-methoxy-2-(4-methoxyphenyl)benzo[β] thiophene (Hauser *et al*, WO 96/30361) with 111 mg (0.58 mmol) 2-naphthoyl chloride was accomplished by the procedure set forth in example **28**(a). The crude product was purified on a chromatotron (silica, 95:5, petroleum ether/ethyl acetate) producing 105 mg (0.25 mmol, 45%) of [2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl][2-naphthyl]methanone as yellow crystals. ¹H nmr (CDCl₃) 8.21 (s, 1H), 7.95 (dd, J = 8.7, 1.7 Hz, 1H), 7.71 (m, 3H), 7.31-7.61 (m, 6H), 6.96 (dd, J = 8.9, 2.5 Hz, 1H), 6.65 (m, 2H), 3.88 (s, 3H), 3.63 (s, 3H).
- (b) The deprotection of 70 mg (0.17 mmol) of [2-(4-methoxyphenyl)-6thien-3-yl][2-naphthyl]methanone (example **29**(a)) methoxybenzo[\beta] was accomplished by the procedure set forth in example 28 (b). The crude product was purified on a chromatotron (silica, 75:25 to 50:50, petroleum ether/ ethyl acetate as 72%) producing 47 m g (0.12)mmol, eluent) gradient [2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][2-naphthyl]methanone as yellow crystals. MP 229-232°C. 'H nmr (CD₃COCD₃) 8.73 (s, 1H), 8.52 (s, 1H), 8.24 (s, 1H), 7.83-7.98 (m, 4H), 7.41-7.63 (m, 4H), 7.22-7.33 (m, 2H), 6.96 (dd, J = 8.8, 2.2 Hz, 1H), 6.65 (m, 2H).

Example 34

[2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-tert-butylphenyl] methanone (30).

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- (a) The acylation of 150 mg, (0.55 mmol) 6-methoxy-2-(4-methoxyphenyl)benzo[β] thiophene (Hauser *et al*, WO 96/30361) with 115 mg (0.58 mmol) 4-tert-butylbenzoyl chloride was accomplished by the procedure set forth in example **28**(a). The crude product was purified on a chromatotron (silica, 95:5, petroleum ether/ethyl acetate) producing 125 mg (0.29 mmol, 52%) of [2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl][4-tert-butylphenyl]methanone as yellow crystals. H nmr (CDCl₃) 7.64-7.73 (m, 2H), 7.55 (d, J = 8.9 Hz, 1H), 7.22-7.34 (m, 5H), 6.95 (dd, J = 8.9, 2.5 Hz, 1H), 6.72 (m, 2H), 3.87 (s, 3H), 3.71 (s, 3H), 1.22 (s, 9H).
- (b) The deprotection of 70 mg (0.17 mmol) 2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl][4-tert-butylphenyl]methanone (example (30a)) was accomplished by the procedure set forth in example 28 (b). The crude product was purified on a chromatotron (silica, gradient 75:25 to 50:50, petroleum ether/ ethyl acetate) producing 30 mg (0.07 mmol, 46%) of [2-(4-hydroxyphenyl)-6-hydroxybenzo[β]thien-3-yl] [4-tert-butylphenyl]methanone as yellow crystals. MP 197-200°C, ¹H nmr (CD₃COCD₃) 8.69 (s, 1H), 8.60 (s, 1H), 7.63-7.70 (m, 2H), 7.35-7.46 (m, 4H), 7.21-7.28 (m, 2H), 6.94 (d, J = 8.8, 2.2 Hz, 1H), 6.72 (m, 2H), 1.28 (s, 9H).

Example 35

[2-(4-hydroxyphenyl)-6-hydroxybenzo[β]thien-3-yl][4-methoxyphenyl]methanone (31).

(a) The acylation of 150 mg, (0.55 mmol) 6-methoxy-2-(4-methoxyphenyl)benzo[β] thiophene (Hauser *et al*, WO 96/30361) with 99 mg (0.58 mmol) 4-methoxybenzoyl chloride was accomplished by the procedure set forth in example **28**(a). The crude product was purified on a chromatotron (silica, 95:5, petroleum ether/ethyl acetate) producing 112 mg (0.27 mmol, 50%) of [2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl][4-methoxyphenyl]methanone as yellow crystals.

(b) The deprotection of 70 mg (0.17 mmol) 2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl][4-methoxyphenyl]methanone(example (31a)) was accomplished by the procedure set forth in example 28 (b). The crude product was purified on a chromatotron (silica, 50:50, petroleum ether/ ethyl acetate) producing 40 mg (0.07 mmol. 63%) of [2-(4-hydroxyphenyl)-6-hydroxybenzo[β]thien-3-yl] [4-methoxyphenyl]methanone as yellow crystals. H nmr (CD₃COCD₃) 8.71 (s, 2H broad), 7.73 (m, 2H), 7.38-7.42 (m, 2H), 7.28(m, 2H), 6.94 (dd, J = 8.4, 2.4 Hz, 1H), 6.86 (m, 2H), 6.75 (m, 2H), 3.79 (s, 3H).

Example 36

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[2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-carboxyphenyl]methanone (32).

- (a) The acylation of 506 mg, (1.87 mmol) 6-methoxy-2-(4-methoxyphenyl)benzo[β] thiophene (Hauser *et al*, WO 96/30361) with 390 mg (1.97 mmol) terephthalic acid monomethyl ester chloride was accomplished by the procedure set forth in example **28**(a). The crude product was purified on a chromatotron (silica, 8:2 petroleum ether/ethyl acetate) producing 442 mg (1.02 mmol, 55%) of [2-(4-ethoxycarbonylphenyl] 6-methoxybenzo[β] thien-3-yl] [4-methoxycarbonylphenyl]methanone.
- (b) The deprotection of 406 mg (0.94 mmol) [2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl][4-methoxycarbonylphenyl]methanone. (example (32a)) was accomplished by the procedure set forth in example 1 (c). The crude product was purified by recrystallisation (acetic acid/ dichloromethane/ methanol) producing 270 mg (0.69 mmol, 73%) of [2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-carboxyphenyl]methanone. H nmr (CD₃COCD₃) 8.76 (s, 1H broad), 8.63 (s, 1H broad), 7.92-7.98 (m, 2H), 7.76-7.83 (m, 2H), 7.63 (d, J = 8.8 Hz, 1H), 7.41 (d, J = 2.5 Hz, 1H), 7.21 (m, 2H), 6.99 (dd, J = 8.8, 2.5 Hz, 1H), 6.69 (m, 2H).

Example 37

[2-(4-hydroxyphenyl)-6-hydroxybenzo[β]thien-3-yl][4-methoxycarbonylphenyl]methanone (33).

[4-carboxyphenyl]methanone (example 32(b)) were dissolved in methanol and five drops of thionyl chloride were added. The reaction mixture was stirred at room temperature for 24 hours, quenched with water, extracted with ethyl acetate and dried over magnesium sulphate. The crude product was purified on a chromatothron (silica, 9:1 petroleum ether/ethyl acetate) producing 42 mg (0.1 mmol, 42%) of $2-(4-h y d r o x y p h e n y 1)-6-h y d r o x y b e n z o [\beta] thien-3-y1][4-methoxycarbonylphenyl]methanone. H nmr (CD₃OD) 8.76 (s, 1H broad), 7.82-7.88 (m, 2H), 7.66-7.72 (m, 2H), 7.61 (d, J = 8.9 Hz, 1H), 7.28 (d, J = 2.4 Hz, 1H), 7.08-7.14 (m, 2H), 6.90 (dd, J = 8.9, 2.4 Hz, 1H), 6.53-6.60 (m, 2H), 3.85 (s, 3H).$

Example 38

[2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-ethoxycarbonylphenyl]methanone (34).

50 mg (0.12 mmol) [2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-carboxyphenyl]methanone (example 32(b)) were dissolved in ethanol and five drops of thionyl chloride were added. The reaction mixture was stirred at room temperature for 24 hours, quenched with water, extracted with ethyl acetate and dried over magnesium sulphate. The crude product was purified on a chromatothron (silica, 9:1 petroleum ether/ethyl acetate) producing 39 mg (0.1 mmol, 74%) of 2-(4-hydroxyphenyl)-6-hydroxybenzo[β]thien-3-yl][4-ethoxycarbonylphenyl]methanone. ¹H nmr (CD₃OD) 8.72 (s, 2H broad), 7.87-7.94 (m, 2H), 7.76-7.82 (m, 2H), 7.62 (d, J = 8.8 Hz, 1H), 7.42 (d, J = 2.2 Hz, 1H), 7.17-7.24 (m, 2H), 6.99 (dd, J = 8.8, 2.2

Hz. 1H), 6.66-6.72 (m, 2H), 4.31 (q, 2H), 1.32 (t, 3H).

Example 39

[2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-cyanophenyl]methanone (35).

- (a) The acylation of 300 mg, (1.11 mmol) 6-methoxy-2-(4-methoxyphenyl)benzo[β] thiophene (Hauser *et al*, WO 96/30361) with 193 mg (1.17 mmol) 4-cyanobenzoyl chloride was accomplished by the procedure set forth in example **28**(a). The crude product was purified on a chromatotron (silica, 8:2 petroleum ether/ethyl acetate) producing 206 mg (0.52 mmol, 46%) of [2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl][4-cyanophenyl]methanone.
- (b) The deprotection of 30 mg (0.075 mmol) [2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl][4-cyanophenyl]methanone (example (35a)) was accomplished by the procedure set forth in example 1 (c). The crude product was purified on a chromatotron (silica, 5:5 petroleum ether/ethyl acetate) producing 24 mg (0.06 mmol, 86%) of [2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-cyanophenyl]methanone. H nmr (CD₃COCD₃) 8.77 (s, 1H broad), 8.73 (s, 1H broad), 7.78-7.85 (m. 2H), 7.65-7.73 (m, 3H), 7.43 (d, J = 2.2 Hz, 1H), 7.16 (m 2H), 7.02, (dd, J = 8.8, 2.2 Hz, 1H), 6.69 (m, 2H).

Example 40

[2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-(1H-tetrazol-5-yl) phenyl]methanone (36).

30 mg (0.08 mmol) [2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-cyanophenyl]methanone (example 35(b)) was dissolved in 1 ml of N, N-dimethylformamide and kept under nitrogen. To the reaction mixture was added 49

mg (0.08 mmol) sodium azide and 40 mg (0.08 mmol) ammonium chloride, then it was heated to reflux temperature for 2 hours. The N, N-dimethylformamide was removed in a speed-vac. The compound was deprotected by the procedure set forth in example 1 (c). The crude product was purified on HPLC (reversed phase, C18, gradient acetonitrile/ water + 0.05 trifluoroacetic acid) producing 24 mg (0.06) mmol, 72%) of [2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-(1H-tetrazol-5-yl) phenyl]methanone. H nmr (CD₃COCD₃) 8.80 (s, 1H), 8.65 (s, 1H), 8.00-8.12 (m, 2H), 7.86-7.92 (m, 2H), 7.62 (d, J = 8.8 Hz, 1H), 7.42 (d, J = 2.2 Hz, 1H), 7.18-7.28, (m, 2H), 7.00 (dd, J = 8.8, 2.2 Hz, 1H), 6.65-6.75 (m, 2H).

Example 41

5-oxo-5-[2-(4-hydroxyphenyl)-6-hydroxybenzo[β]thien-3-yl]pentanoic acid methyl ester (37).

- (a) The acylation of 200 mg, (0.74 mmol) 6-methoxy-2-(4-methoxyphenyl)benzo[β] thiophene (Hauser *et al*, WO 96/30361) with 139 mg (0.78 mmol) methyl adipoyl chloride was accomplished by the procedure set forth in example **28**(a). The crude product was purified on a chromatotron (silica, 9:1 petroleum ether/ethyl acetate) producing 91 mg (0.22 mmol, 30%) of 5-oxo-5-[2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl]pentanoic acid methyl ester.
- (b) The deprotection of 80 mg (0.19 mmol) 5-oxo-5-[2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl]pentanoic acid methyl ester (example (37a)) was accomplished by the procedure set forth in example 1 (c). The crude product was purified on a chromatotron (silica, 98:2 chloroform/methanol + acetic acid) producing 38 mg (0.10 mmol, 52%) of 5-oxo-5-[2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl]pentanoic acid methyl ester. ¹H nmr (CD₃COCD₃) 8.86 (s, 1H broad), 8.67 (s, 1H broad), 7.82 (d, J = 8.8 Hz, 1H), 7.28-7.40 (m, 3H), 6.95-7.05 (m 3H), 3.56 (s, 3H), 2.37-2.46 (m, 2H), 2.11-2.20 (m, 2H), 1.36-1.60 (m, 4H).

Example 42

5-oxo-5-[2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl]pentanoic acid (38).

25 mg (0.06 mmol) of 5-oxo-5-[2-(4-hydroxyphenyl)-6-hydroxybenzo[β]thien-3-yl] pentanoic acid methyl ester (example 37(b) was dissolved in five ml of methanol and 0.5 ml of 1 M sodium hydroxide. The reaction mixture was stirred for one hour, neutralized, extracted with ethyl acetate and dried over magnesium sulphate. This produced 11 mg (0.03 mmol, 49%) of 5-oxo-5-[2-(4-hydroxyphenyl)-6-hydroxybenzo[β]thien-3-yl]pentanoic acid. H nmr (CD₃COCD₃) 7.82 (d, J = 8.8 Hz, 1H), 7.28-7.40 (m, 3H), 6.90-7.05 (m 3H).

Example 43

[2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-propylphenyl]methanone (39).

- (a) The acylation of 200 mg, (0.74 mmol) 6-methoxy-2-(4-methoxyphenyl)benzo[β] thiophene (Hauser *et al*, WO 96/30361) with 142 mg (1.17 mmol) 4-propylbenzoyl chloride was accomplished by the procedure set forth in example 28(a). The crude product was purified on a chromatotron (silica, 9:1 petroleum ether/ethyl acetate) producing 128 mg (0.52 mmol, 42%) of [2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl][4-isopropylphenyl]methanone.
- (b) The deprotection of 100 mg (0.24 mmol) [2-(4-methoxyphenyl)-6-methoxybenzo [β]thien-3-yl][4-isopropylphenyl]methanone.

(example (39a)) was accomplished by the procedure set forth in example 1 (c). The crude product was purified on a chromatotron (silica, 5:5 petroleum ether/ethyl acetate) producing 28 mg (0.07 mmol, 30%) of [2-(4-hydroxyphenyl)-6-hydroxybenzo [β]thien-3-yl][4-propylphenyl]methanone. H nmr (CD₃COCD₃) 8.71 (s, 1H), 8.62 (s, 1H), 7.62-7.70 (m, 2H), 7.45 (d, J = 8.8 Hz, 1H), 7.39 (d, J = 2.2 Hz, 1H), 7.21-7.28

(m 2H), 7.14-7.20 (m, 2H), 6.94, (dd, J = 8.8, 2.2 Hz, 1H), 6.68-6.75 (m, 2H), 2.55 (t, 2H), 1.58 (m, 2H), 0.88 (t, 3H).

Example 44

[2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-iodophenyl]methanone (40).

- a) The acylation of 200 mg, (0.74 mmol) 6-methoxy-2-(4-methoxyphenyl)benzo[β] thiophene (Hauser *et al*, WO 96/30361) with 207 mg (0.77 mmol) 4-iodobenzoyl chloride was accomplished by the procedure set forth in example **28**(a). The crude product was purified on a chromatotron (silica, 9:1 petroleum ether/ethyl acetate) producing 258 mg (0.52 mmol, 70%) of [2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl][4-iodophenyl]methanone.
- (b) The deprotection of 100 mg (0.20 mmol) [2-(4-methoxyphenyl)-6-methoxybenzo [β]thien-3-yl][4-iodophenyl]methanone.

(example (40)) was accomplished by the procedure set forth in example 1 (c). The crude product was purified on a chromatotron (silica, 5:5 petroleum ether/ethyl acetate) producing 43 mg (0.09 mmol, 45%) of [2-(4-hydroxyphenyl)-6-hydroxybenzo[β]thien-3-yl][4-iodophenyl]methanone. ¹H nmr (CD₃COCD₃) 8.71 (s, 2H, broad), 8.62 (s, 1H), 7.69-7.78 (m, 2H), 7.54 (d, J = 8.8 Hz, 1H), 7.45-7.50 (m, 2H), 7.40 (d, J = 2.2 Hz, 1H), 7.17-7.24 (m 2H), 6.96, (dd, J = 8.8, 2.2 Hz, 1H), 6.68-6.75 (m, 2H).

Example 45

2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-acetylphenyl]methanone (41).

(a) A mixture of 246 mg (0.75 mmol) of hexamethylditin, 250 mg (0.50 mmol) of

[2-(4-methoxyphenyl)-6-methoxybenzo[β]thien-3-yl][4-iodophenyl] methanone. (example (39a)), 6 mg (0.005 mmol)) tetrakis triphenylphosphinepalladium (0) and 20 ml toluene was heated under reflux in a nitrogen atmosphere for 20 h. The reaction mixture was concentrated, dissolved in diethylether, washed with water twice, dried over magnesium sulphate, filtered and concentrated. This yielded 241 mg (0.45 mmol, 90%) of the desired [2-(4-methoxyphenyl)-6-methoxybenzo[β]thien-3-yl][4-trimethylstannylphenyl]methanone.

(b) 100 mg (0.19 mmol) of [2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl][4-trimethylstannylphenyl]methanone (example 41(a)) and 15 mg (0.19 mmol) of acetyl chloride was dissolved in 5 ml of toluene. To the reaction mixture was added 4.6 mg (0.0044 mmol) of tris(dibenzylideneacetone)palladium(0)*chloroform. The reaction mixture was then heated under a nitrogen atmosphere at 70⑤ C 20 hours, filtered, extracted with ethyl acetate, washed with saturated sodium bicarbonate and dried over magnesium sulphate. The deprotection of the crude [2-(4-methoxyphenyl)-6-methoxybenzo[β]thien-3-yl][4-acetylphenyl]methanone was accomplished by the procedure set forth in example 1 (c). The product was purified on a chromatotron (silica, 5:5 petroleum ether/ethyl acetate) producing 61 mg (0.16 mmol, 82%) of [2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-acetylphenyl]methanone. ¹H nmr (CD₃COCD₃) 7.85-7.92 (m, 2H), 7.76-7.83 (m, 2H), 7.59 (d, J = 8.8 Hz, 1H), 7.41 (d, J = 2.2 Hz, 1H), 7.17-7.24 (m 2H), 6.98, (dd, J = 8.8, 2.2 Hz, 1H), 6.66-6.73 (m, 2H), 2.54 (s, 3H).

Example 46

2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-propionylphenyl]methanone (42).

200 mg (0.38 mmol) of [2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl][4-trimethylstannylphenyl]methanone (example 41(a)) and 34 mg (0.38 mmol) of propionyl chloride was dissolved in 10 ml of toluene. To the reaction mixture was

added 9.2 mg (0.0088 mmol) of tris(dibenzylideneacetone)palladium(0)*chloroform. The reaction mixture was then heated under a nitrogen atmosphere at 70°C for 20 hours, filtered, extracted with ethyl acetate, washed with saturated sodium bicarbonate and dried over magnesium sulphate. The deprotection of the crude [2-(4-methoxyphenyl)-6-methoxybenzo[β]thien-3-yl][4-propionylphenyl]methanone was accomplished by the procedure set forth in example 1 (c). The crude product was purified on HPLC (reversed phase, C18, gradient acetonitrile/ water + 0.05 trifluoroacetic acid) producing 9 mg (0.02 mmol, 6%) of [2-(4-hydroxyphenyl)-6-hydroxybenzo[β]thien-3-yl][4-propionylphenyl]methanone. H nmr (CD₃COCD₃) 8.72 (s, 1H), 8.61 (s, 1H), 7.85-7.92 (m, 2H), 7.76-7.83 (m, 2H), 7.59 (d, J = 8.8 Hz, 1H), 7.41 (d, J = 2.2 Hz, 1H), 7.17-7.24 (m 2H), 6.98, (dd, J = 8.8, 2.2 Hz, 1H), 6.66-6.73 (m, 2H), 2.99 (q, 2H), 1.08 (t. 3H).

Example 47

2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-buturylphenyl]methanone (43).

100 mg (0.19 mmol) of [2-(4-methoxyphenyl)-6-methoxybenzo[β]thien-3-yl][4-trimethylstannylphenyl]methanone (example 41(a)) and 22 mg (0.20 mmol) of buturyl chloride was dissolved in 5 ml of toluene. To the reaction mixture was added 4.6 mg (0.0044 mmol) of tris(dibenzylideneacetone)palladium(0)*chloroform. The reaction mixture was then heated under a nitrogen atmosphere at 70°C for 20 hours, filtered, extracted with ethyl acetate, washed with saturated sodium bicarbonate and dried over magnesium sulphate. The crude product was purified on a chromatotron (silica, 9:1 petroleum ether/ethyl acetate). The deprotection of the crude [2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl][4-buturylphenyl]methanone was accomplished by the procedure set forth in example 1 (c). The product was purified on a chromatotron (silica, 9:1 petroleum ether/ethyl acetate) producing 17 mg (0.04 mmol, 22%) of [2-(4-hydroxyphenyl)-6-hydroxybenzo[β]thien-3-yl][4-buturylphenyl]methanone. ¹H nmr (CD₁COCD₃) 8.72 (s, 1H), 8.61 (s, 1H), 7.85-7.92 (m, 2H), 7.76-7.83 (m, 2H),

7.60 (d, J = 8.8 Hz, 1H), 7.42 (d, J = 2.2 Hz, 1H), 7.17-7.24 (m 2H), 6.99, (dd, J = 8.8, 2.2 Hz, 1H), 6.66-6.73 (m, 2H), 2.96 (q, 2H), 1.67 (m, 2H), 1.08 (t. 3H).

Example 48

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[2-(4-hydroxyphenyl)-6-hydroxybenzo[β]thien-3-yl][4-ethylthiocarbonylphenyl]-methanone (44).

mg (0.12 mmol) [2-(4-hydroxyphenyl)-6-hydroxybenzo[β]thien-3-yl][4-carboxyphenyl]methanone (example 32(b)) were dissolved in ethanthiol and five drops of thionyl chloride were added. The reaction mixture was stirred at room temperature for 24 hours in a nitrogen atmosphere, quenched with water, extracted with ethyl acetate and dried over magnesium sulphate. The crude product was purified on HPLC (reversed phase, C18, gradient acetonitrile/ water + 0.05 trifluoroacetic acid) producing 26 mg (0.06 mmol, 54%) of 2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-ethylthiocarbonylphenyl]methanone. ¹H nmr (CD₃OD) 8.72 (s, 1H broad), 8.60 (s, 1H), 7.89-7.98 (m, 2H), 7.75-7.84 (m, 2H), 7.61 (d, J = 8.8 Hz, 1H), 7.42 (d, J = 2.5 Hz, 1H), 7.17-7.24 (m, 2H), 6.99 (dd, J = 8.8, 2.5 Hz, 1H), 6.66-6.72 (m, 2H), 2.89 (q, 2H), 1.32 (t, 3H).

Example 49

2-(4-hydroxyphenyl)-6-hydroxybenzo[β khien-3-yl][4-hydroxyphenyl]methanone (45)

The deprotection of 2-(4-methoxyphenyl)-6-methoxybenzo[β]thien-3-yl][4-methoxyphenyl]methanone (example (31a)) as described in example 31(b) produced after purification 2-(4-hydroxyphenyl)-6-hydroxybenzo[β]thien-3-yl][4- hydroxyphenyl]methanone as a byproduct. H nmr (CD₃COCD₃) 8.60-9.00 (s, 3H broad), 7.62-7.72 (m, 2H), 7.36-7.40 (m, 2H), 7.22-7.28 (m, 2H), 6.92 (dd, J = 8.6, 2.4 Hz, 1H), 6.68-6.80 (m, 4H).

Example 50

2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-methylamino carbonyl-phenyl]methanone (46)

2-(4-methoxyphenyl)-6-methoxybenzo[\beta] thien-3-yl][4-methoxycarbonylphenyl]methanone (example 32(b)) was deprotected to 2-(4-methoxyphenyl)-6-methoxybenzo[\beta] thien-3-yl][4-carboxyphenyl]methanone by dissolving in ethanol and stirring with 1M sodium hydroxide for 4 hours. The ethanol was evaporated and the aqueous phase was extracted with ethylacetate, dried over magnesium sulphate and evaporated. The following reaction was run in a parallell solution phase way. 20 mg (0.048 mmol) of 2-(4-methoxyphenyl)-6-methoxybenzo[β] thien-3-yl][4-carboxyphenyl]methanone was mixed in sequential order with 30 mg (0.058 mmol) of benzotriazole-1-yl-oxy-tris-pyrrolidino-phosphonium hexafluorophosphate (PyBOP), 3.6 mg (0.024 mmol) of N-hydroxybenzotriazole*H₂O (HOBt), 2.5 ml of N,N-dimethylformylamide, 12.4 mg (0.096 mmol) of N,N-diisopropylethylamine and 2.23 mg (0.096 mmol) of methylamine hydrochloride in a nitrogen atmosphere at room-temperature for 3 days. The reaction was diluted with ethyl acetate. The organic phase was washed with 10% citric acid, dried by passing through a 3 ml extube. Varian Chem. Elut, and concentrated on a speed-vac. The deprotection of 2-(4-methoxyphenyl)--6-methoxybenzo[β] thien-3-yl][4-methylaminocarbonylphenyl]methanone as described in example 1(c) produced after purification on HPLC (reversed phase, C18, gradient acetonitrile/ water + 0.05 trifluoroacetic acid) 6 mg (0.015 mmol, 31%) of 2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-methylaminophenyl]methanone. 'H nmr (CD₃COCD₃) 7.70-7.85 (m, 4H), 7.55 (d, J = 8.8, 1H), 7.41 (d, J = 2.2, 1H), 7.19-7.25 (m, 2H), 6.99 (d, J = 8.8, 2.2 Hz, 1H), 6.66-6.74 (m, 2H).

Example 51

 $2-(4-hydroxyphenyl)-6-hydroxybenzo[\beta]$ thien-3-yl][4-isobutylaminocarbonylphenyl]methanone (47)

This reaction was run in a parallell solution phase way by the procedure set forth in example 46, using isobutylamine hydrochloride (5.24 mg (0.096 mmmol)) instead of methylamine. The crude product was purified on HPLC (reversed phase, C18, gradient acetonitrile/ water + 0.05 trifluoroacetic acid) producing 1.2 mg (0.0027 mmol, 5.6 %) of 2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-isobutylaminophenyl]-methanone. ¹H nmr (CD₃COCD₃) 7.72-7.92 (m, 4H), 7.51 (d, J = 8.8, 1H), 7.42 (d, J = 2.2 Hz, 1H), 7.18-7.26 (m, 2H), 6.97 (dd, J = 8.8, 2.2 Hz, 1H), 6.66-6.76 (m, 2H).

Example 52

2 - $(4 - h y d r o x y p h e n y l) - 6 - h y d r o x y b e n z o [\beta] thien - 3 - y l] - [4-benzylaminocarbonylphenyl]methanone (48)$

This reaction was run in a parallell solution phase way by the procedure set forth in example 46, using benzylamine hydrochloride (7.68 mg (0.096 mmol) instead of methylamine. The crude product was purified on HPLC (reversed phase, C18, gradient acetonitrile/ water + 0.05 trifluoroacetic acid) producing 1.7 mg (0.0035 mmol, 7.4 %) of 2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-bensylaminophenyl]-methanone. ¹H nmr (CD₃COCD₃) 8.33 (s, broad), 7.85-7.91 (m, 2H), 7.75-7.82 (m, 2H), 7.53 (d, J = 8.8 Hz, 1H), 7.42 (d, J = 2.2 Hz, 1H), 7.18-7.36 (m, 7H), 6.98 (dd, J = 8.8, 2.2 Hz, 1H), 6.68-6.74 (m, 2H).

Example 53

15 mg (0.040 mmol) of 2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-carboxyphenyl]methanone (example 32(b)) was mixed in sequential order with 40 mg (0.077 mmol) of benzotriazole-1-yl-oxy-tris-pyrrolidino-phosphonium hexafluoro-phosphate (PyBOP), 4.9 mg (0.032 mmol) of N-hydroxybenzotriazole*H₂O (HOBt),

3.0 ml of *N*,*N*-dimethylformylamide, 16.5 mg (0.128 mmol) of N,N-diisopropylethylamine and 0.015 g (0.096 mmol) of L-serine methylester hydrochloride in a nitrogen atmosphere at room-temperature for 3 days. The reaction was diluted with ethyl acetate. The organic phase was washed with 1M hydrochloric acid and brine. Then dried over magnesium sulphate and evaporated to dryness. Purification on HPLC (reversed phase, C18, gradient acetonitrile/ water + 0.05 trifluoroacetic acid) produced 7.4 mg (0.015 mmol, 38%) of 49. ¹H nmr (CD₃COCD₃) 7.78-7.92 (m, 4H), 7.55 (d, J = 8.8, 1H), 7.41 (d, J = 2.2, 1H), 7.19-7.28 (m, 2H), 6.98 (dd, J = 8.8, 2.2 Hz, 1H), 6.66-6.74 (m, 2H), 4.69 (m, 1H), 3.95 (m, 2H), 3.69 (s, 3H).

Example 54

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15 mg (0.040 mmol) of 2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-carboxyphenyl]methanone (example 32(b)) was mixed in sequential order with 40 mg (0.077 mmol) of benzotriazole-1-yl-oxy-tris-pyrrolidino-phosphonium hexafluoro-phosphate (PyBOP), 4.9 mg (0.032 mmol) of N-hydroxybenzotriazole*H₂O (HOBt), 3.0 ml of N,N-dimethylformylamide, 16.5 mg (0.128 mmol) of N,N-diisopropylethylamine and 0.013 g (0.096 mmol) of L-alanine methylester hydrochloride in a nitrogen atmosphere at room-temperature for 3 days. The reaction was diluted with ethyl acetate. The organic phase was washed with 1M hydrochloric acid and brine. Then dried over magnesium sulphate and evaporated to dryness. Purification on HPLC (reversed phase, C18, gradient acetonitrile/ water + 0.05 trifluoroacetic acid) produced 17.4 mg (0.037 mmol, 91%) of 50. ¹H nmr (CD₃COCD₃) 8.12 (s, 1H broad), 8.10 (s, 1H broad), 7.75-7.89 (m, 4H), 7.53 (d, J = 8.8, 1H), 7.41 (d, J = 2.2, 1H), 7.17-7.23 (m, 2H), 6.98 (dd, J = 8.8, 2.2 Hz, 1H), 6.69-6.74 (m, 2H), 4.59 (m, 1H), 3.66 (s, 3H), 1.45 (d, 3H).

Example 55

15 mg (0.040 mmol) of 2-(4-hydroxyphenyl)-6-hydroxybenzo[β] thien-3-yl][4-carboxyphenyl]methanone (example 32(b)) was mixed in sequential order with 40 mg

(0.077 mmol) of benzotriazole-1-yl-oxy-tris-pyrrolidino-phosphonium hexafluoro-phosphate (PyBOP), 4.9 mg (0.032 mmol) of N-hydroxybenzotriazole*H₂O (HOBt), 3.0 ml of N.N-dimethylformylamide, 16.5 mg (0.128 mmol) of N,N-diisopropylethylamine and 0.021 g (0.096 mmol) of L-phenylalanine methylester hydrochloride in a nitrogen atmosphere at room-temperature for 3 days. The reaction was diluted with ethyl acetate. The organic phase was washed with 1M hydrochloric acid and brine. Then dried over magnesium sulphate and evaporated to dryness. Purification on HPLC (reversed phase, C18, gradient acetonitrile/ water + 0.05 trifluoroacetic acid) produced 10.9 mg (0.020 mmol, 51%) of 51. H nmr (CD₃COCD₃) 8.01 (s, 1H broad), 7.98 (s, 1H broad), 7.75 (s, 4H), 7.53 (d, J = 8.8, 1H), 7.41 (d, J = 2.2, 1H), 7.15-7.31 (m, 7H), 6.98 (dd, J = 8.8, 2.2 Hz, 1H), 6.69-6.74 (m, 2H), 4.82 (m, 1H), 3.65 (s, 3H).

The biological character of the compounds prepared in accordance with Examples 1 to 26 and 28 to 40 inclusive and also, for comparison purposes estradiol was measured in a radioligand displacement assay. The affinity for ER α and ER β was measured as an IC₅₀, the concentration of ligand necessary to displace 50% of tritated 17- β -estradiol from either hER α (human estrogen receptor α) or hER β (human estrogen receptor β) respectively. In this assay, it was found that the IC₅₀'s of compounds varied from 2.0 nM to 20 μ M for ER α and from 2.0 nM to 12 μ M for ER β . The ER α /ER β selectivity ratio varied from 0.2 to 23.

Experimental description of ER binding assay

Affinity for the ER (by displacement of ³[H]-estradiol) ws measured using the scintistrip assay¹. Human estrogen receptors (hER) alpha and beta were extracted from the nuclei from SF9-cells infected with a recombinant baculovirus transfer vector containing the cloned hER genes.² The concentration of hER's in the extract was measured as specific ³[H]-E2 binding with the G25-assay.³

- 1) Haggblad, J., Carlsson, B., Kivelä, P., Siitari, H., (1995) Biotechniques 18, 146-151.
- 2) Barkhem, T., Carlsson, B., Simons, J., Moller, B., Berkenstam, A., Gustafsson

- J.A.G., Nilsson, S. (1991) J. Steroid Biochem. Molec. Biol. 38, 667-75.
- 3) Salononsson, M., Carlsson, B., Haggblad, J., (1994) J. Steroid Biochem. Molec. Biol. 50, 313-318.

CLAIMS

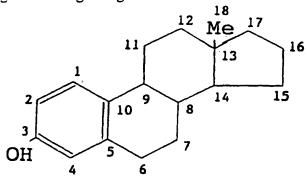
- 1. A crystal comprising at least a portion of the ERα ligand binding domain.
- 2. A crystal according to claim 1 comprising at least 200 amino acids of ERα.
- 3. A crystal according to claim 1 or claim 2 comprising at least 250 amino acids of ERα.
- 4. A crystal according to claim 1,2 or 3 comprising entire ERa.
- 5. A crystal according to any preceding claim produced using a sequence including helix $H_{\rm to}$ of $ER\alpha$.
- 6. A crystal according to any one of claims 1 to 5 usable in X-ray crystallography techniques.
- 7. A crystal according to any one of claims 1 to 6 including a ligand bound to $ER\alpha$ or a portion thereof.
- 8. A crystal according to claim 7 in which the ligand is estradiol, raloxifene, or any other ligand that binds with high affinity ($<10\mu M$) to ER α .
- 9. A crystal of ERα LBD according to any preceding claim belonging to the space group P2, and having the unit cell dimensions a=61.48Å, b=115.16Å, c=137.38Å.
- 10. A crystal of ER α LBD according to any preceding claim belonging to the space group P2 and having the unit cell dimensions a=104.53Å b=53.68Å c=102.71Å and β =116.79°.
- 11. A crystal of ERa LBD according to any one of claims 1 to 9 belonging to the

space group C2 and having the unit cell dimensions a=89.91Å b=75.09Å c=87.50Å and β =103.01°.

- 12. A crystal of ERα LBD according to any one of claims 1 to 9 belonging to the space group C222₁ and having the unit cell dimensions a=65.47Å b=95.99Å c=164.14Å.
- 13. A method for designing ligands which will bind to an estrogen receptor, the method comprising determining amino acid or acids of the ligand binding domain of the estrogen receptor which interact with a binding ligand, and selecting a ligand which is likely to bind to the receptor according to the structure of the potential ligand.
- 14. A method according to claim 13 in which interaction with ER α and ER β are separately determined whereby ER-form selective ligands can be selected.
- 15. A method according to claim 13 or 14, in which for ERα selective ligands the design of the potential ligand uses a crystal according to any one of claims 1 to 12.
- 16. Ligands for estrogen receptors designed using a method according to claim 13, 14 or 15.
- 17. Ligands designed according to a method according to claim 14 which are specific for ER α or ER β .
- 18. Ligands binding to at least the LBD of an ER with an affinity of between 20 pmol and 200 nM.
- 19. Ligands binding reversibly to at least the LBD of an ER.
- 20. A method of inhibiting estadiol activity in an animal, the method comprising

administering to the animal a ligand according to claim 19 or claim 20.

- 21. A method of inhibiting estradiol activity according to claim 20 comprising administering a ligand according to claim 18 or claim 19.
- 22. A pharmaceutical compound comprising a ligand according to any one of claims 16 to 19.
- 23. An estrogen agonist, an estrogen antagonist, a partial estrogen agonist, or a partial estrogen antagonist designed using a method according to claim 13, 14 or 15.
- 24. An ER α selective ligand having a structural group larger than methyl capable of fitting into the β cavity of the ER α .
- 25. An ERa selective ligand having the general formula Z



and having hydrophobic substituents at one or more of the 8β ,15 β or 18 positions.

- 26. An ER β selective ligand having the formula Z of claim 25 and having hydrophobic substituents at one or more of the 9α or 12α positions.
- 27. An ERα selective ligand according to claim 25 or ERβ selective ligand according to claim 26 in which the hydrophobic substituent is selected from methyl groups, ethyl groups, iso-propyl groups, chlorine, bromine or iodine.
- 28. An ERα or ERβ selective ligand, in which the ligand is a 2'-,3'-.5'- and/or 6'-

substituted 2-aryl benzothiophene.

- 29. An ER α or ER β selective ligand according to claim 28, which is substituted at one or more of the 2',3', 5' and 6' positions.
- 30. An ER α selective ligand according to claim 28, in which the substituted 2-aryl benzothiophene fills the α and β -face cavities of the ER.
- 31. An ER α selective ligand, which is a 2-aryl benzotheiphene with a small hydrophobic substituent at one or more of the 2',3',5' and 6' positions.
- 32. An ER ligand capable of filling the hydrophobic cavity of ER-α.
- 33. A ligand according to claim 32 which has a hydrophobic substituent on the ethoxyphenyl sidechain to the piperidinyl nitrogen atom of raloxifene.
- 34. A ligand according to claim 31 or 32 in which the ligand has a hydrophobic sustituent selected from linear alkyl groups, perfluoroalkyl groups (-CH₃ to -CH₁₀H₂₁, -CF₃ to -C₁₀F₂₁), benzyl-(CH₂Ph), benzyl-(methylene cyclohexyl groups).
- 35. An ER ligand having a structure capable of interacting with Glu-353 of ER α or with Glu-262 of ER β .
- 36. An ER ligand having a structure capable of interacting with Arg-394 of ER α or with Arg-303 or ER β .
- 37. An ER ligand having a structure capable of interacting with residue His-524 of $ER\alpha$ or with His-432 of $ER\beta$.
- 38. An ER ligand having a structure capable of interacting with Met-421 or Leu-384 of ER α or with Ile-330 Met-293 of ER β .

- 39. An ER α selective ligand having a structure capable of interacting with Met-421 and/or Leu-384 of ER α .
- 40. An ER β selective ligand having a structure capable of interaction with Ile-330 and/or Met-293 of ER β .
- 41. An ER β selective ligand according to claim 40 in which substitutions larger than a methyl group are provided at the α 14,16 or 17 positions of the steroid nucleus.
- 42. An ER ligand having a structure capable of interacting with Leu-384 of ER α or Met-293 of ER β .
- 43. An ERα selective ligand capable of interacting with Leu-384 of ERα.
- 44. An ERβ selective ligand capable of interacting with Met-293 of ERβ.
- 45. An ERβ selective ligand according to claim 40 further provided with substituents at the 2° or 3° positions of the 2-aryl benzothiophene nucleus.
- 46. An ER β selective ligand having a substituent larger than a methyl group at the R₂' position of a 6.3'-dihydroxybenzothiophene.
- 47. An ER α selective ligand having a substituent larger than a methyl group at either the R₂ and/or R₃ position of a 6,5'-dihydroxybenzothiophene.
- 48. A ligand selective for either ER α or ER β in which the ligand comprises a position-6 substituent from the benzothiophene nucleus or position-3 substituent from the estradiol nucleus arranged to selectively bind to either the amino acid Ile-326 of ER α or Asn-236 of ER β .
- 49. A ligand selective for either ERα or ERβ in which the ligand comprises a

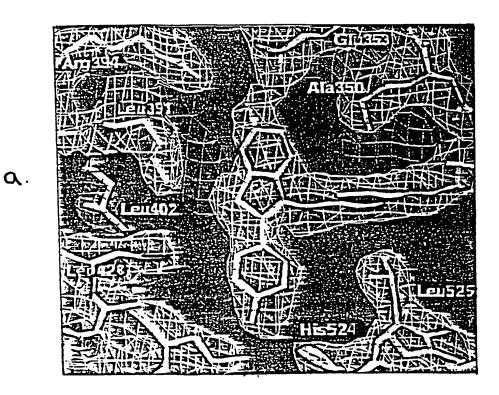
position-6 substituent from the benzothiophene nucleus or position-3 substituent from the estradiol nucleus arranged to selectively bind to either the amino acid Phe-445 of $ER\alpha$ or Tyr-354 of $ER\beta$.

- 50. An ER α selective ligand having a structure capable of simultaneously interacting with Glu-323 and Phe-445 of ER α in preference to Glu-262 and Tyr-354 of ER β .
- 51. An ER ligand having a structure arranged to promote binding with Helix H12 of the ER structure.
- 52. A crystal according to any of claims 1 to 12, having a resolution determined by X-ray crystallography less than 3.5Å.
- 53. A machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a crystal according to any one of claims 1 to 12 or a homologue of said crystal.
- 54. A method for evaluating the ability of a chemical entity to associate with an estrogen receptor, the method comprising the steps of:
- a) employing computational means to perform a fitting operation between the chemical entity and a binding site of the receptor; and
- b) analysing the results of the fitting operation to predict the association between the chemical entity and the binding site.
- 55. A crystallized molecule or molecular complex comprising a binding pocket defined by the structure coordinates of human ER-α ligand binding domain amino acid residues MET343, LEU346, THR347. LEU349, ALA350, ASP351, GLU353, LEU354, TRP383, LEU384, LEU387, MET388, LEU391, ARG394, PHE404, MET421, ILE424,

- PHE425, LEU428, GLY521, HIS524, LEU525 or a homologue of said molecule or molecular complex, wherein said homologue has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.
- 56. A homology model comprising a binding pocket defined by the structure coordinates of human ER-β ligand binding domain amino acid residues MET343, LEU346. THR347. LEU349, ALA350, ASP351, GLU353, LEU354, TRP383, MET384. LEU387. MET388, LEU388, LEU391, ARG394, PHE404, ILE421, ILE424, PHE425, LEU428. GLY521, HIS524, LEU525.
- 57. A crystallized molecule or molecular complex comprising a binding pocket defined by the structure coordinates of rat ER-α ligand binding domain amino acid residues MET252, LEU255, THR256, LEU258, ALA259, ASP260, GLU262, LEU263, TRP292, LEU293, LEU296, MET297, LEU300, ARG303, PHE313, ILE330, IL333, PHE334, LEU337, GLY429, HIS423, LEU433 or a homologue of said molecule or molecular complex, wherein said homologue has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.
- 58. A homology model comprising a binding pocket defined by the structure coordinates of rat ER-β ligand binding domain amino acid residues MET252, LEU255. THR256. LEU258, ALA259, ASP260, GLU262, LEU263, TRP292, MET293, LEU296, MET297, LEU300, ARG303, PHE313, ILE330, ILE333, PHE334, LEU337, GLY429, HIS432, LEU433.
- 59. A method of agonising or antagonising ER α or ER β , the method comprising administering to a mammal a compound, other than raloxifene, that fits spatially into the binding pocket of ER β .
- 60. A method according to claim 59 in which the compounds has at least one of the following:
 - a group capable of functioning as a hydrogen bond donor to HIS432;

- b) A group that functions as a hydrogen bond acceptor and donor to Arg-394 and Glu-353 of ERα or Arg-303 and Glu-262 of ERβ;
- c) a group capable of forming a hydrophobic contact with at least one of Met-252, Leu-255, Leu-258, Ala-259, Leu-263, Trp-292, Met-293, Leu-296, Met-297, Leu-300, Phe-313, Ile-330, Ile-333, Phe-334, Leu-337, Leu-433 of ERβ, or Met-343, Leu-346, Leu-349, Ala-350, Leu-354, Trp-383, Leu-384, Leu-387, Met-388, Leu-391, Phe-404, Met-421, Ile-424, Phe-425, Leu-428, Leu-525, of ERα.
- 61. A method of antagonising ER β according to claim 59 or 60 in which the compound has a group that can form either a hydrogen bond or a salt bridge to ASP260.
- 62. A method of antagonising ER α according to claim 59 or 60 in which the compound has a group that can form either a hydrogen bond or a salt bridge to Asp-351.
- 63. An ER ligand in accordance with any one of the Examples 5 to 55.

FIGURE 1



Ь.

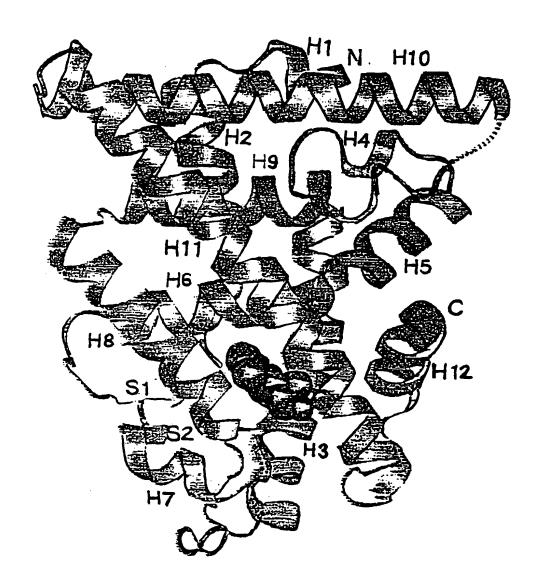
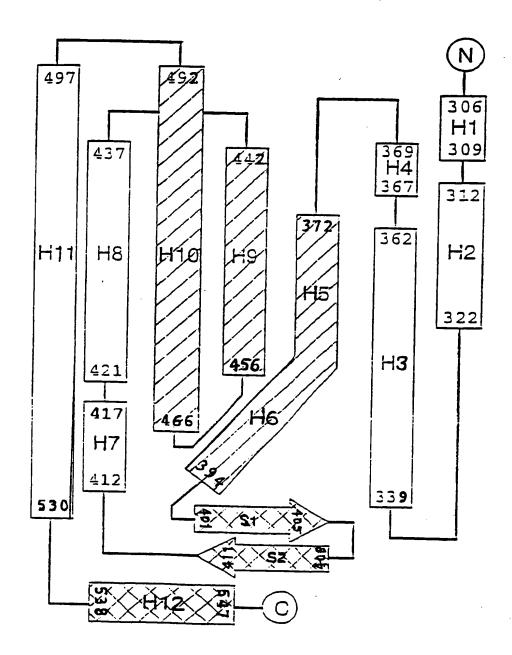


FIGURE 2a

FIGURE 2b





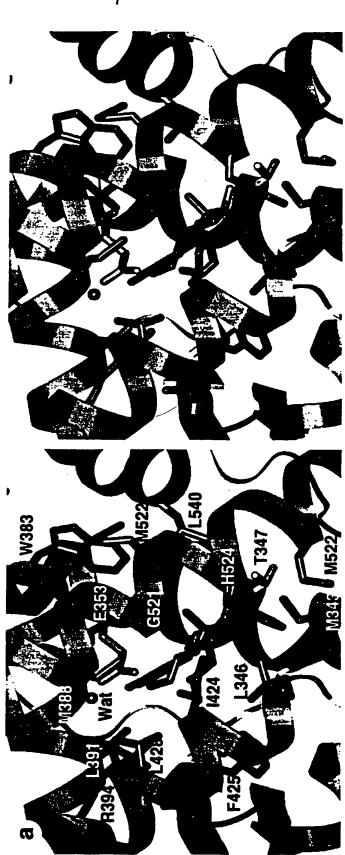
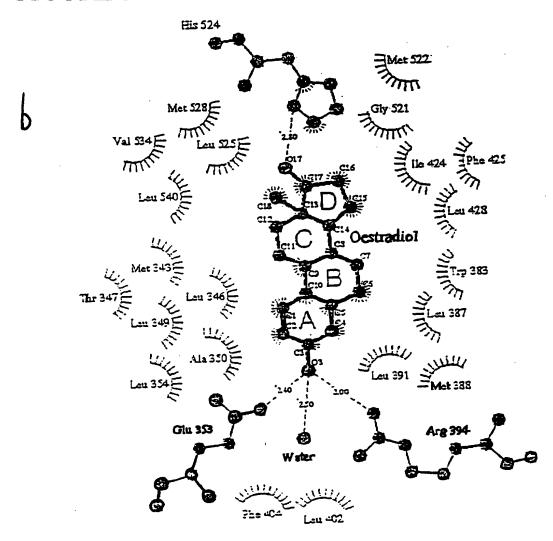
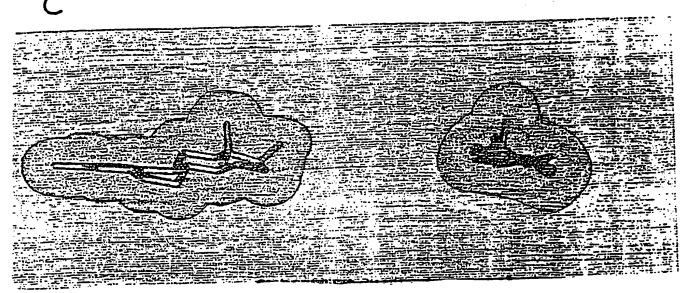


FIGURE 3

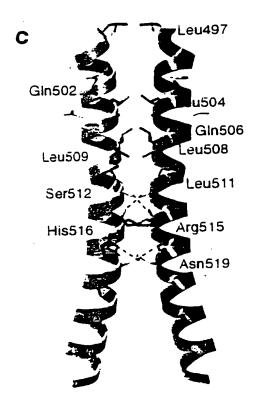


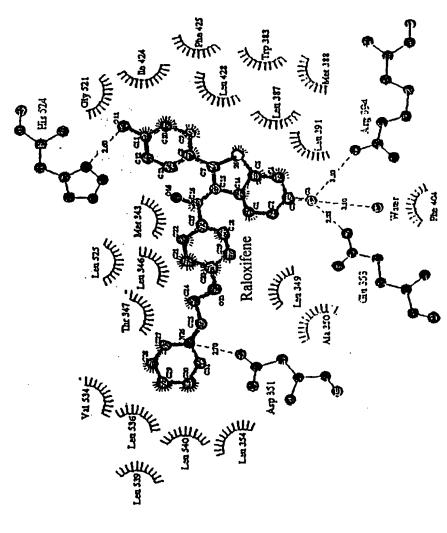


SUBSTITUTE SHEET (RULE 26)

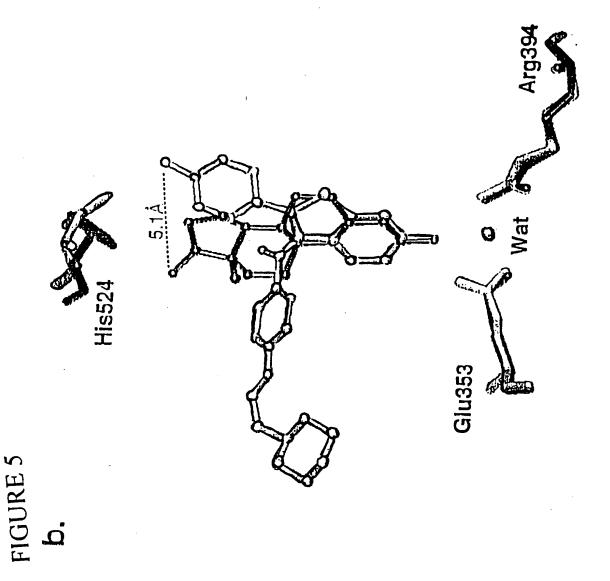


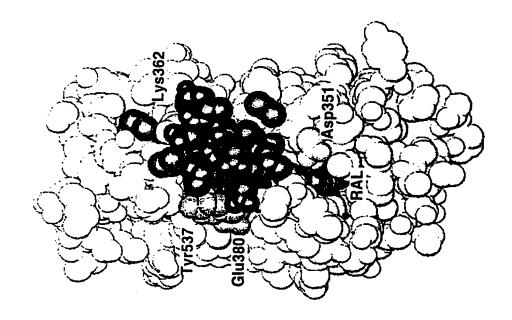
FIGURE 4





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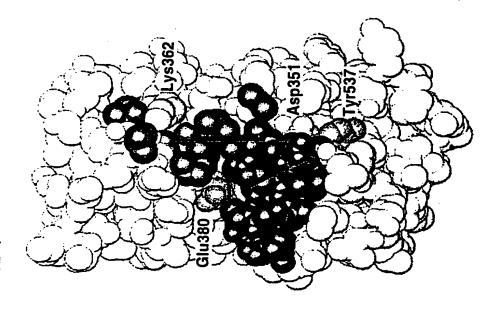
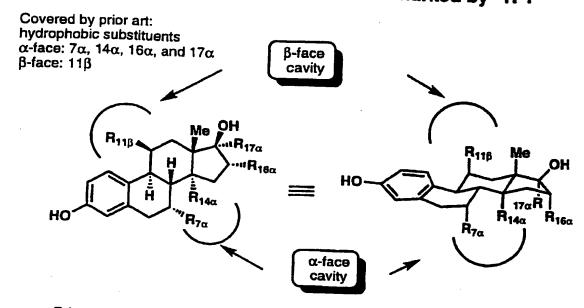


FIGURE 7

FIGURE 8

Zearalenone

Figure 8a: affinity enhancing substituents marked by "R".



Prior art reviewed in "The estradiol pharmacophore: ligand structure-estrogen receptor binding affinity relationships" G.M. Anstead, K.E. Carlson, and J.A. Katzenellenbogen, Steroids, 62(3):268-303 (1997).

Figure 8b: affinity enhancing substituents marked by "R".

Not covered by prior art: hydrophobic substituents
$$\alpha$$
-face: 9α and 12α β -face: 8β , 15β , and 18 $R_{12\alpha}$ R_{18} R_{19} R_{19}

Figure 8c: affinity enhancing substituents marked by "R".

Figure 8d: affinity enhancing substituents. Replacement of 4'-OH group in raloxifene with 4'-NH₂ provides the opportunity of picking up an additional hydrogen bond to His-524.

Figure 8e: guanidino affinity enhancing substituent at position-3 of the steroid nucleus and position-6 of the benzothiophene nucleus.

Figure 9a: selectivity enhancing substituents R₃, R₂', R₃', and R₆'.

$$\alpha$$
-face Lew/Met-384

Ho R₃ R₂' R₃' His-524

 β -face Met/Ile-421

 R_3 , R_2 ', R_3 ', and R_6 ' = Cl, Br, I, Me, Et, *i*-Pr, and perfluoro Me, Et, and *i*-Pr.

Figure 9b: selectivity enhancing substituents R_3 , R_2 ', R_3 ', and R_6 '. Movement of hydroxyl from position-4' to -5' biases binding orientation and therefore further enhances selectivity.

 R_3 , R_2 ', R_3 ', and R_6 ' = Cl, Br, I, Me, Et, *i*-Pr, and perfluoro Me, Et, and *i*-Pr.

Figure 9c: selectivity enhancing substituents R₃.

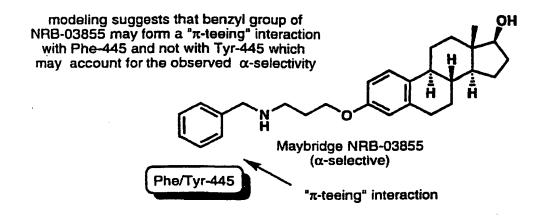


Figure 9d: selectivity enhancing substituents R₆.

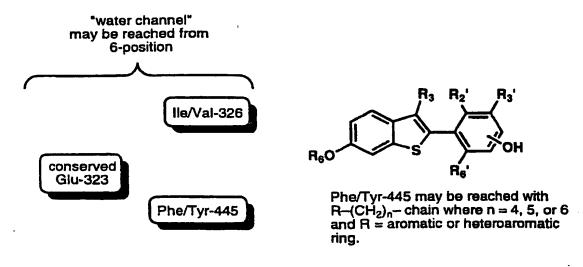
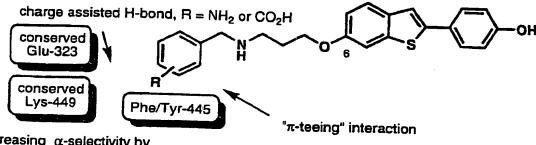


Figure 9e: selectivity enhancement reinforced by charged assisted hydrogen bond betwen substitutient "R" in the ligand and either Glu-323 or Lys-449 in the receptor.



Increasing α-selectivity by reinforcing Phe-445 interaction with H-bonding to Glu-323

Figure 9f: selectivity enhancement reinforced by hydrogen bond network between pyridone ring in the ligand and residues Glu-323 and Lys-449 in the receptor.

FIGURE 10

25, 25, 24, 25, 15, 17, 17, 15, 11, 11, 11, 11, 10, 9, 7, 6, 5, 4, 5, 6, 2, 11, 12, 13, 14, 15, 14, 15, 14, 15

FIGURE 10 continued



FIGURE 11

Example 16,18

FIGURE 12

FIGURE 13

Example 22

FIGURE 14

Example 28, 29, 30, 31, 32, 35, 37, 38, 39, 40, 45

FIGURE 15

FIGURE 16

FIGURE 17

Example 41, 42, 43

FIGURE 18

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Example 46, 47, 48

FIGURE 19

Example 49, 50, 51

FIGURE 20

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08-SEP-97 1ERR HEADER NUCLEAR RECEPTOR COMPND MOL_ID: 1; COMPND 2 MOLECULE: OESTROGEN RECEPTOR; COMPND 3 CHAIN: A, B; COMPND 4 FRAGMENT: LIGAND-BINDING DOMAIN; COMPND 5 SYNONYM: ESTROGEN RECEPTOR, ER-LBD; COMPND 6 ENGINEERED: YES; COMPND 7 BIOLOGICAL_UNIT: DIMER; COMPND 8 OTHER_DETAILS: LIGAND-BINDING DOMAIN COMPND 9 (DOMAIN E - RESIDUES 301-553) IN COMPLEX WITH THE **SELECTIVE** COMPND 10 ANTAGONIST RALOXIFENE SOURCE MOL ID: 1; SOURCE 2 ORGANISM SCIENTIFIC: HOMO SAPIENS; SOURCE 3 ORGANISM_COMMON: HUMAN; SOURCE 4 STRAIN: JM109; SOURCE 5 VARIANT: C1857; SOURCE 6 PLASMID: PEALPHA 35; SOURCE 7 GENE: ER ALPHA; SOURCE 8 EXPRESSION SYSTEM: ESCHERICHIA COLI; SOURCE 9 EXPRESSION_SYSTEM_STRAIN: JM109; SOURCE 10 EXPRESSION SYSTEM_VARIANT: C1857; SOURCE 11 EXPRESSION SYSTEM PLASMID: PEALPHA 35 AUTHOR A.M.BRZOZOWSKI, A.C.W.PIKE JRNL AUTH A.M.BRZOZOWSKI, A.C.W.PIKE, Z.DAUTER, R.E.HUBBARD, JRNL AUTH 2 T.BONN, O.ENGSTROM, L.OHMAN, G.L. GREENE, JRNL AUTH 3 J.-A. GUSTAFFSON, M. CARLQUIST JRNL TITL MOLECULAR BASIS OF AGONISM AND ANTAGONISM IN THE JRNL TITL 2 OESTROGEN RECEPTOR JRNL REF TO BE PUBLISHED 0353 IRNL REFN ASTM REMARK 1 REMARK 2 REMARK 2 RESOLUTION. 2.6 ANGSTROMS. REMARK 3 REMARK 3 REFINEMENT. REMARK 3 PROGRAM : REFMAC REMARK 3 AUTHORS : MURSHUDOV, VAGIN, DODSON REMARK 3 REMARK 3 DATA USED IN REFINEMENT. REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS): 2.6 REMARK 3 RESOLUTION RANGE LOW (ANGSTROMS): 25 REMARK 3 DATA CUTOFF (SIGMA(F)): 0 REMARK 3 COMPLETENESS FOR RANGE (%): 95.7 : 15433 REMARK 3 NUMBER OF REFLECTIONS REMARK 3

REMARK 3 FIT TO DATA USED IN REFINEMENT.

REMARK 3 CROSS-VALIDATION METHOD : THROUGHOUT REMARK 3 FREE R VALUE TEST SET SELECTION: RANDOM REMARK 3 R VALUE (WORKING + TEST SET): NONE

REMARK 3 R VALUE (WORKING SET): 0.219

REMARK 3 FREE R VALUE : 0.299

REMARK 3 FREE R VALUE TEST SET SIZE (%): 10 REMARK 3 FREE R VALUE TEST SET COUNT : 1565

REMARK 3

REMARK 3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.

REMARK 3 PROTEIN ATOMS : 3553 REMARK 3 NUCLEIC ACID ATOMS REMARK 3 HETEROGEN ATOMS : 80 REMARK 3 SOLVENT ATOMS : 100

REMARK 3 REMARK 6

REMARK 6 ER-LBD WAS CARBOXYMETHYLATED PRIOR TO

CRYSTALLISATION, ONLY

REMARK 6 THE CARBOXYMETHYL GROUP BOUND TO CYS 381 COULD BE CLEARLY

REMARK 6 LOCATED IN THE MAPS. THIS GROUP IS PRESENTED IN THE

REMARK 6 COORDINATE FILE AS HET GROUP CBM 381 AT THE END OF EACH

REMARK 6 CHAIN.

REMARK 7

REMARK 7 RESIDUES TYR331(A), ASP332(A), HIS377(B), GLU397(AB),

REMARK 7 LYS416(AB), GLU419(AB), GLU423(B), LEU469(B), GLU470(AB), GLU471

REMARK 7 (AB),LYS472(AB),ARG477(AB),LYS492(A),LYS529(B),GLU542(A),

REMARK 7 ARG548(B) AND LEU549(B) WERE POORLY RESOLVED IN THE ELECTRON

REMARK 7 DENSITY MAPS AND ARE NOT FULLY MODELLED IN THIS ENTRY.

REMARK 8

REMARK 8 RESIDUES MODELLED IN ALTERNATE CONFORMATIONS: A373, A377,

REMARK 8 A381,A473,A501,B455-B457,B501,B526.

REMARK 999

REMARK 999 SEQUENCE

REMARK 999 REFERENCE: SER A 301 - LEU A 306 MISSING FROM PDB DUE TO DISORDER

REMARK 999 REFERENCE: THR A 460 - LEU A 469 MISSING FROM PDB DUE TO DISORDER

REMARK 999 REFERENCE: LYS A 529 - VAL A 534 MISSING FROM PDB DUE TO DISORDER

REMARK 999 REFERENCE: ARG A 548 - THR A 553 MISSING FROM PDB DUE TO DISORDER

0

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REMARK 999 REFERENCE: SER B 301 - SER B 305 MISSING FROM PDB DUE TO DISORDER REMARK 999 REFERENCE: ASP B 332 - GLU B 339 MISSING FROM PDB DUE TO DISORDER REMARK 999 REFERENCE: THR B 460 - SER B 468 MISSING FROM PDB DUE TO DISORDER REMARK 999 REFERENCE: CYS B 530 - PRO B 535 MISSING FROM PDB DUE TO DISORDER REMARK 999 REFERENCE: PRO B 552 - THR B 553 MISSING FROM PDB DUE TO DISORDER SG ACYS A 381 LINK C2 ACBM A 381 SG BCYS A 381 LINK C2 ACBM A 381 SG ACYS A 381 C2 BCBM A 381 LINK SG BCYS A 381 LINK C2 BCBM A 381 SG CYS B 381 C2 CBM B 381 LINK CISPEP | ARG A 335 PRO A 336 0 0.13 CRYST1 104.530 53.680 102.710 90.00 116.79 90.00 C 1 2 1 ORIGX1 1.000000 0.000000 0.000000 0.00000 0.000000 1.000000 0.000000 0.00000 ORIGX2 0.000000 0.000000 1.000000 0.00000 ORIGX3 SCALE 1 0.009567 0.000000 0.004830 0.00000 0.000000 0.018629 0.000000 0.00000 SCALE2 0.000000 0.000000 0.010907 0.00000 SCALE3 MTRIX1 1 -0.740953 -0.502251 0.445794 74.86100 1 MTRIX2 1 -0.502316 -0.026089 -0.864290 122.90400 1 MTRIX3 1 0.445721 -0.864328 -0.232958 94.95000 1 1 N ALA A 307 54.098 63.501 73.107 1.00101.44 N ATOM C 2 CA ALA A 307 53.995 62.069 72.653 1.00101.06 ATOM 3 C ALA A 307 52.966 61.945 71.536 1.00100.17 C ATOM 0 4 O ALA A 307 53.280 61.646 70.377 1.00 99.09 ATOM 5 CB ALA A 307 53.690 61.140 73.815 1.00100.89 C ATOM N 6 N LEU A 308 51.722 62,276 71.868 1.00 99.53 ATOM C 50.596 62.259 70.953 1.00 99.09 7 CA LEU A 308 ATOM C 50.516 63.528 70.121 1.00 98.93 8 C LEU A 308 ATOM 0 49.540 63.825 69.426 1.00100.59 9 O LEU A 308 ATOM 49.302 62.048 71.772 1.00 98.27 C 10 CB LEU A 308 ATOM C 49.294 60.672 72.455 1.00 98.34 11 CG LEU A 308 ATOM C 48,270 60,564 73,564 1,00 99,10 ATOM 12 CD1 LEU A 308 C 49.073 59.608 71.396 1.00 99.05 ATOM 13 CD2 LEU A 308 N 51.593 64.289 70.149 1.00 97.52 14 N SER A 309 ATOM 51.799 65.546 69.479 1.00 94.74 C 15 CA SER A 309 ATOM C 52.762 65.407 68.308 1.00 90.63 ATOM 16 C SER A 309 53.020 66.365 67.590 1.00 91.89 0 ATOM 17 O SER A 309 C 52.357 66.583 70.456 1.00 96.58 18 CB SER A 309 ATOM 0 52.346 66.102 71.800 1.00100.04 ATOM 19 OG SER A 309 53.298 64.214 68.092 1.00 85.74 N 20 N LEU A 310 ATOM C 54.212 64.025 66.973 1.00 80.17 21 CA LEU A 310 ATOM 53.475 63.652 65.701 1.00 75.60 C 22 C LEU A 310 ATOM

23 O LEU A 310

52.519 62.877 65.644 1.00 75.27

ATOM

		•	
ATOM	24 CB LEU A 310	55.259 62.961 67.314 1.00 82.19	С
ATOM	25 CG LEU A 310	56.128 63.380 68.513 1.00 84.04	С
ATOM	26 CD1 LEU A 310	56,916 62.196 69.021 1.00 85.21	С
ATOM	27 CD2 LEU A 310	57.028 64.542 68.119 1.00 85.94	С
ATOM	28 N THR A 311	53.925 64.277 64.620 1.00 69.23	N
ATOM	29 CA THR A 311	53.347 64.005 63.307 1.00 65.09	С
ATOM	30 C THR A 311	53.830 62.585 62.954 1.00 61.00	С
ATOM	31 O THR A 311	54.838 62.147 63.496 1.00 56.82	0
ATOM	32 CB THR A 311	53.884 64.913 62.189 1.00 66.58	С
ATOM	33 OG1 THR A 311	55.198 64.441 61.861 1.00 67.83	0
ATOM	34 CG2 THR A 311	53.990 66.380 62.503 1.00 66.63	С
ATOM	35 N ALA A 312	53.190 62.002 61.942 1.00 59.73	N
ATOM	36 CA ALA A 312	53.629 60.694 61.475 1.00 56.36	С
ATOM	37 C ALA A 312	55.145 60.754 61.272 1.00 55.33	C
ATOM	38 O ALA A 312	55.871 59.918 61.816 1.00 55.73	0
ATOM	39 CB ALA A 312	53.021 60.320 60.154 1.00 55.64	С
ATOM	40 N ASP A 313	55.562 61.758 60.497 1.00 55.51	N
ATOM	41 CA ASP A 313	57.000 61.809 60.232 1.00 61.36	С
ATOM	42 C ASP A 313	57.854 62.030 61.457 1.00 60.56	С
ATOM	43 O ASP A 313	58.925 61.401 61.501 1.00 59.92	Ο
ATOM	44 CB ASP A 313	57.421 62.678 59.065 1.00 66.00	С
ATOM	45 CG ASP A 313	56.760 62.221 57.760 1.00 70.36	C
ATOM	46 OD1 ASP A 313	57.126 61.157 57.216 1.00 69.20	0
ATOM	47 OD2 ASP A 313	55.822 62.967 57.358 1.00 73.76	O
ATOM	48 N GLN A 314	57.425 62.794 62.443 1.00 61.07	N
ATOM	49 CA GLN A 314	58.238 63.006 63.637 1.00 63.62	С
ATOM	50 C GLN A 314	58.386 61.687 64.414 1.00 60.76	С
ATOM	51 O GLN A 314	59.476 61.412 64.904 1.00 60.44	Ο
ATOM	52 CB GLN A 314	57.673 64.099 64.529 1.00 68.68	С
ATOM	53 CG GLN A 314	57.411 65.462 63.876 1.00 72.34	С
ATOM	54 CD GLN A 314	56.582 66.319 64.835 1.00 75.22	С
ATOM	55 OE1 GLN A 314	55.389 66.117 65.001 1.00 74.32	0
ATOM	56 NE2 GLN A 314	57.215 67.294 65.498 1.00 76.79	N
ATOM	57 N MET A 315	57.321 60.921 64.486 1.00 57.60	N
ATOM	58 CA MET A 315	57.248 59.628 65.129 1.00 54.58	С
ATOM	59 C MET A 315	58.322 58.723 64.541 1.00 52.34	С
ATOM	60 O MET A 315	59.175 58.099 65.180 1.00 49.28	0
ATOM	61 CB MET A 315	55.852 59.057 64.781 1.00 59.63	С
ATOM	62 CG MET A 315	55.573 57.619 65.179 1.00 61.37	C
ATOM	63 SD MET A 315	55.131 57.546 66.947 1.00 67.38	S
ATOM	64 CE MET A 315	56.797 57.583 67.603 1.00 65.02	С
ATOM	65 N VAL A 316	58.280 58.672 63.198 1.00 49.88	N
ATOM	66 CA VAL A 316	59.184 57.774 62.491 1.00 50.51	С
ATOM	67 C VAL A 316	60.656 58.049 62.696 1.00 49.96	С
ATOM	68 O VAL A 316	61.451 57.091 62.811 1.00 50.67	0
ATOM	69 CB VAL A 316	58.854 57.823 60.983 1.00 52.04	С
ATOM	70 CG1 VAL A 316	59.711 56.828 60.214 1.00 51.77	С
ATOM	71 CG2 VAL A 316	57.367 57.602 60.863 1.00 50.35	С
ATOM	72 N SER A 317	61.003 59.331 62.639 1.00 48.06	N

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ATOM		2.423 59.721 62.777 1.00 48.67	С
ATOM	74 C SER A 317 62.	.813 59.525 64.238 1.00 47.57	С
ATOM	75 O SER A 317 63	.778 58.816 64.595 1.00 48.05	О
ATOM	76 CB SER A 317 62	2.430 61.196 62.364 1.00 49.56	С
ATOM	77 OG SER A 317 6	1.339 61.700 63.181 1.00 54.05	О
ATOM	78 N ALA A 318 62	2.000 60.024 65.158 1.00 43.79	N
ATOM	79 CA ALA A 318 6	2.259 59.753 66.577 1.00 42.79	С
ATOM	80 C ALA A 318 62	2.622 58.278 66.738 1.00 46.07	C
ATOM	81 O ALA A 318 63	3.724 57.937 67.164 1.00 48.86	0
ATOM	82 CB ALA A 318 6	0.958 60.040 67.312 1.00 43.54	С
ATOM	83 N LEU A 319 61	1.721 57.372 66.259 1.00 44.84	N
ATOM	84 CA LEU A 319 6	1.958 55.967 66.457 1.00 39.49	С
ATOM	85 C LEU A 319 63	.249 55,560 65,808 1.00 41.35	С
ATOM	86 O LEU A 319 64	1.114 54.940 66.442 1.00 43.08	O
ATOM		0.818 55.095 66.132 1.00 35.20	С
ATOM		9,455 55,190 66,778 1,00 34,47	С
ATOM		58.471 54.330 65.923 1.00 33.78	С
ATOM		59.388 54.770 68.217 1.00 28.80	С
ATOM		3.462 55.915 64.567 1.00 46.80	N
ATOM		4.721 55.511 63.886 1.00 48.28	С
ATOM		5,946 55,905 64,667 1,00 49,61	С
ATOM		5.922 55.170 64.714 1.00 50.99	Ο
ATOM		4.715 56.108 62.472 1.00 48.30	С
ATOM		53.875 55.286 61.483 1.00 49.80	С
ATOM		63,709 55,967 60.158 1.00 49.05	С
ATOM	,	64.519 53.925 61.255 1.00 51.04	С
ATOM		5.935 57.068 65.308 1.00 53.09	N
ATOM		57.033 57.589 66.105 1.00 53.45	С
ATOM		7.294 56.752 67.337 1.00 48.52	С
ATOM		8.447 56.506 67.654 1.00 52.66	Ο
ATOM		66.739 59.000 66.649 1.00 57.98	С
ATOM		67.872 59.919 66.255 1.00 63.89	С
ATOM		68.362 59.817 65.107 1.00 66.13	0
ATOM		68.276 60.724 67.122 1.00 69.06	0
ATOM		66.228 56.278 67.943 1.00 41.85	N
ATOM		66.295 55.442 69.123 1.00 36.67	С
ATOM		66.794 54.049 68.847 1.00 33.38	С
ATOM		56.970 53.238 69.749 1.00 34.81	0
ATOM		64.909 55.394 69.764 1.00 36.73	С
ATOM		57.078 53.724 67.616 1.00 31.88	N
ATOM		67.392 52.340 67.287 1.00 34.43	С
ATOM		68.526 51.925 68.094 1.00 35.40	С
ATOM	• • • • • • • • • • • • • • • • • • • •	59.427 52.756 68.242 1.00 44.66	0
ATOM		67.529 52.209 65.773 1.00 35.17	С
ATOM		66.158 51.707 65.178 1.00 38.58	С
ATOM		65.893 50.295 65.659 1.00 39.26	C
ATOM		66.456 49.328 65.149 1.00 42.62	0
ATOM	120 OE2 GLU A 323	65.132 50.082 66.607 1.00 42.24	O
		58.537 50.780 68.697 1.00 37.20	N
ATOM	IAL IN FIXUA 324 U	0,557 50,760 00,057 1.00 57.20	

	_ ·		
ATOM	122 CA PRO A 324	69.755 50.328 69.431 1.00 37.25	С
ATOM	123 C PRO A 324 7	0.811 50.012 68.373 1.00 37.44	С
ATOM	124 O PRO A 324 7	0.483 49.787 67.218 1.00 38.76	Ο
ATOM	125 CB PRO A 324	69.416 49.034 70.128 1.00 33.21	С
ATOM	126 CG PRO A 324	68.160 48.636 69.459 1.00 33.49	С
ATOM	127 CD PRO A 324	67.551 49.752 68.621 1.00 34.65	С
ATOM	128 N PRO A 325 7	2.044 49.948 68.804 1.00 36.23	N
ATOM	129 CA PRO A 325	73.174 49.603 67.970 1.00 34.39	С
ATOM	130 C PRO A 325 7	3.223 48.132 67.679 1.00 36.48	С
ATOM	131 O PRO A 325 7	2.707 47.405 68.550 1.00 43.04	. 0
ATOM	• •	74.395 49.931 68.883 1.00 30.34	С
ATOM	133 CG PRO A 325	73.826 49.651 70.222 1.00 33.20	С
ATOM	134 CD PRO A 325	72.412 50.153 70.200 1.00 35.18	С
ATOM	135 N ILE A 326 73	3.844 47.574 66.682 1.00 37.00	N
ATOM	136 CA ILE A 326 7	3.891 46.094 66.592 1.00 35.96	С
ATOM	137 C ILE A 326 75	5.121 45.635 67.301 1.00 39.02	С
ATOM	138 O ILE A 326 76	5.214 46.058 66.903 1.00 47.09	Ο
ATOM	139 CB ILE A 326 7	3.877 45,664 65.119 1.00 37.18	С
ATOM	140 CG1 ILE A 326	72.440 45.960 64.571 1.00 33.71	С
ATOM		74.228 44.209 64.877 1.00 34.30	С
ATOM		72.322 45.838 63.110 1.00 32.65	С
ATOM		75.061 44.831 68.339 1.00 38.76	N
ATOM		76.223 44.386 69.099 1.00 33.89	C
ATOM	• • • • • • •	6.869 43.164 68.493 1.00 37.30	C
ATOM		76.300 42.514 67.653 1.00 35.59	0
ATOM	- · · · · · · · · · · · · · · · ·	75.761 44.038 70.533 1.00 31.03	C
ATOM	• • • • •	75.027 45.176 71.259 1.00 31.56	C
ATOM		74.951 44.900 72.762 1.00 28.63	C
ATOM	150 CD2 LEU A 327	75.747 46.531 71.068 1.00 29.79	C
ATOM		78.065 42.777 68.973 1.00 39.80	N
ATOM	•	78.752 41.596 68.506 1.00 38.44	C
ATOM		78.791 40.517 69.572 1.00 42.46	C O
ATOM	••••	78.752 40.739 70.808 1.00 40.42 80.223 41.999 68.242 1.00 39.84	C
ATOM	155 CB TYR A 328 156 CG TYR A 328	80.429 42.530 66.862 1.00 44.53	C
ATOM		80.133 43.840 66.561 1.00 46.24	C
ATOM	157 CD1 T1R A 328 158 CD2 TYR A 328	80.912 41.696 65.840 1.00 48.79	C
ATOM ATOM	150 CD2 TTR A 328	80.305 44.316 65.284 1.00 50.15	C
ATOM	160 CE2 TYR A 328	81.078 42.159 64.556 1.00 49.24	C
ATOM	161 CZ TYR A 328	80.754 43.475 64.302 1.00 52.20	c
ATOM	161 CZ TTRA 328	80.907 44.010 63.033 1.00 59.80	o
ATOM		79.057 39.298 69.107 1.00 45.70	N
ATOM		79.214 38.169 70.008 1.00 51.02	Ċ
ATOM		30.586 38.188 70.668 1.00 56.51	c
ATOM		31.548 38.612 70.018 1:00 55.49	Ö
ATOM		79.156 36.880 69.159 1.00 50.86	C
ATOM	- · · - ·	79.310 35.775 70.062 1.00 52.63	ŏ
ATOM		80.706 37.683 71.878 1.00 65.75	N
ATOM	170 CA GLU A 330	82.025 37.611 72.521 1.00 76.01	C
AT OM	170 CIL GDO 11330	02.020 57.011 72.021 1.00 70.01	_

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ATOM	171 C GLU A 330	82.960 37.133 71.396 1.00 81.00	С
ATOM	172 O GLU A 330	82.675 36.107 70.813 1.00 79.13	Ο
ATOM	173 CB GLU A 330	82.071 36.616 73.647 1.00 79.87	С
ATOM	174 CG GLU A 330	80.998 36.670 74.700 1.00 84.53	С
ATOM	175 CD GLU A 330	81.061 35.563 75.738 1.00 88.62	C
ATOM	176 OE1 GLU A 330	80.793 34.362 75.470 1.00 88.61	Ο
ATOM	177 OE2 GLU A 330	81.382 35.913 76.917 1.00 89.74	Ο
ATOM	178 N TYR A 331	83,985 37,902 71,102 1,00 91,50	N
ATOM	179 CA TYR A 331	84.918 37.609 70.032 1.00100.48	С
ATOM	180 C TYR A 331	85.340 36.141 70.038 1.00107.14	С
ATOM	181 O TYR A 331	85,517 35,555 71.101 1.00108.63	Ο
ATOM		86.138 38.522 70.026 1.00 99.32	. C
ATOM	190 N ASP A 332		N
ATOM	191 CA ASP A 332	85,796 34.214 68.578 1.00120.41	С
ATOM	192 C ASP A 332	86.261 33.397 69.761 1.00124.62	С
ATOM	193 O ASP A 332		0
ATOM	194 CB ASP A 332	86.895 34.137 67.490 1.00120.22	С
ATOM	198 N PRO A 333	•	N
ATOM	199 CA PRO A 333		С
ATOM	200 C PRO A 333		С
ATOM	201 O PRO A 333		0
ATOM	202 CB PRO A 333		С
ATOM		83.390 31.669 71.139 1.00129.68	С
ATOM		83.944 32.552 70.043 1.00128.77	С
ATOM	205 N THR A 334	85,516 29,556 70,526 1,00130,47	N
ATOM	206 CA THR A 334	85.948 28.337 69.884 1.00129.25	С
ATOM	207 C THR A 334	84.785 27.632 69.178 1.00127.54	С
ATOM	208 O THR A 334		O
ATOM	209 CB THR A 334		С
ATOM	210 OG1 THR A 334		0
ATOM	211 CG2 THR A 334		С
ATOM		85.107 27.111 67.999 1.00125.90	N
ATOM	213 CA ARG A 335		С
ATOM	214 C ARG A 335	84.728 25.036 66.825 1.00119.67	C
ATOM	215 O ARG A 335	85.940 24.931 66.633 1.00119.78	Ö
ATOM	216 CB ARG A 335	83.720 27.231 66.009 1.00125.31	C
ATOM		82.285 27.149 65.540 1.00127.03	C
ATOM		81.655 28.529 65.578 1.00128.25	Č
ATOM	219 NE ARG A 335	82.347 29.451 64.686 1.00129.98	N
ATOM	220 CZ ARG A 335	81,682 30.315 63.921 1.00130.52	С
ATOM	221 NH1 ARG A 335		N
ATOM			N
ATOM	223 N PRO A 336	83.912 24.016 66.729 1.00115.59	N
ATOM		82.489 24.100 66.951 1.00113.40	C
ATOM		82.114 24.304 68.410 1.00111.16	C
ATOM	•	82.732 23.804 69.352 1.00110.30	ŏ
ATOM	227 CB PRO A 336	81.900 22.777 66.413 1.00113.87	C
ATOM	228 CG PRO A 336	83.075 21.850 66.561 1.00113.87	Č
ATOM		84.336 22.658 66.384 1.00114.86	Ċ
V T T OTAT	LL, CD INGRUSO	1.0011	

230 N PHE A 337 81.056 25.072 68.653 1.00108.59 N **ATOM** 231 CA PHE A 337 80.592 25.302 70.005 1.00107.41 C **ATOM** ATOM 232 C PHE A 337 79.944 24.019 70.544 1.00105.98 С 233 O PHE A 337 79.608 23.095 69.811 1.00105.97 0 ATOM C 234 CB PHE A 337 79.494 26.381 70.074 1.00108.40 ATOM 79.786 27.668 69.384 1.00109.05 C ATOM 235 CG PHE A 337 80.817 28.477 69.826 1.00110.21 ATOM 236 CD1 PHE A 337 C ATOM 237 CD2 PHE A 337 79.061 28.082 68.283 1.00109.60 C ATOM 238 CE1 PHE A 337 81.137 29.655 69.173 1.00110.99 ATOM 239 CE2 PHE A 337 79.344 29.276 67.646 1.00110.17 C C ATOM 240 CZ PHE A 337 80.379 30.077 68.098 1.00110.36 79.684 24.056 71.839 1.00104.12 N ATOM 241 N SER A 338 ATOM 242 CA SER A 338 78.921 23.005 72.510 1.00101.32 C C ATOM 243 C SER A 338 77.542 23.619 72.828 1.00 99.90 77.245 24.736 72.394 1.00 98.36 ATOM 244 O SER A 338 0 ATOM 245 CB SER A 338 79.628 22.537 73.768 1.00 99.85 C ATOM 246 OG SER A 338 79.630 23.506 74.795 1.00 98.71 0 247 N GLU A 339 76.720 22.900 73.575 1.00 98.70 ATOM N C ATOM 248 CA GLU A 339 75.412 23.419 73.948 1.00 97.01 ATOM 249 C GLU A 339 75.629 24.565 74.947 1.00 92.79 C ATOM 250 O GLU A 339 75.146 25.676 74.716 1.00 91.77 0 ATOM 251 CB GLU A 339 74.542 22.333 74.539 1.00101.76 C ATOM 252 CG GLU A 339 73.174 22.808 75.040 1.00106.56 C C ATOM 253 CD GLU A 339 72.364 21.658 75.609 1.00109.74 254 OE1 GLU A 339 72.856 20.503 75.549 1.00112.97 0 ATOM 71.247 21.895 76.114 1.00110.41 ATOM 255 OE2 GLU A 339 0 ATOM 256 N ALA A 340 76.455 24.326 75.964 1.00 87.20 N ATOM 257 CA ALA A 340 76.727 25.362 76.943 1.00 84.40 C ATOM 258 C ALA A 340 77.497 26.557 76.397 1.00 81.16 C ATOM 259 O ALA A 340 77.234 27.697 76.785 1.00 80.26 0 77.457 24.787 78.161 1.00 85.04 C ATOM 260 CB ALA A 340 ATOM 261 N SER A 341 78.452 26.338 75.510 1.00 77.03 N ATOM 262 CA SER A 341 79.267 27.403 74.926 1.00 72.02 C 78.435 28.351 74.080 1.00 67.47 C ATOM 263 C SER A 341 ATOM 264 O SER A 341 78.568 29.576 74.162 1.00 63.26 0 ATOM 265 CB SER A 341 80.428 26.784 74.137 1.00 71.53 C ATOM 266 OG SER A 341 80.507 27.178 72.795 1.00 69.57 0 ATOM 267 N MET A 342 77.581 27.768 73.248 1.00 64.08 N ATOM 268 CA MET A 342 76.671 28.553 72.431 1.00 62.01 C ATOM 269 C MET A 342 C 75.663 29.290 73.319 1.00 58.62 ATOM 270 O MET A 342 75.325 30.455 73.098 1.00 56.39 0 ATOM 271 CB MET A 342 75.893 27.597 71.535 1.00 62.67 C ATOM 272 CG MET A 342 74.882 28.258 70.647 1.00 63.17 C S ATOM 273 SD MET A 342 74.747 27.389 69.098 1.00 70.28 C ATOM 274 CE MET A 342 73.064 26.783 69.114 1.00 66.11 ATOM 275 N MET A 343 75.190 28.560 74.346 1.00 52.89 N ATOM 276 CA MET A 343 74.213 29.182 75.229 1.00 50.63 C ATOM 277 C MET A 343 74.848 30.415 75.855 1.00 49.91 C 0 ATOM 278 O MET A 343 74.196 31.460 75.988 1.00 52.56

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ATOM	279 CB MET A 343	73.619 28.255 76.258 1.00 50.93	C
ATOM	280 CG MET A 343	72.421 27.408 75.889 1.00 53.30	С
ATOM	281 SD MET A 343	71.438 28.002 74.494 1.00 60.64	S
ATOM	282 CE MET A 343	70.677 29.482 75.224 1.00 52.97	C
ATOM	283 N GLY A 344	76.090 30.324 76.252 1.00 46.32	N
ATOM	284 CA GLY A 344	76.894 31.341 76.853 1.00 40.89	C
ATOM	285 C GLY A 344	77.069 32.501 75.904 1.00 41.62	С
ATOM	286 O GLY A 344	76.845 33.648 76.313 1.00 43.99	Ο
ATOM	287 N LEU A 345	77.379 32.229 74.635 1.00 40.05	N
ATOM	288 CA LEU A 345	77.512 33.370 73.724 1.00 39.66	С
ATOM	289 C LEU A 345	76.152 34.018 73.593 1.00 42.22	С
ATOM	290 O LEU A 345	75.967 35.236 73.827 1.00 40.01	0
ATOM	291 CB LEU A 345	78.094 32.904 72.411 1.00 40.52	С
ATOM	292 CG LEU A 345	79.509 32.281 72.578 1.00 36.81	C
ATOM	293 CD1 LEU A 345	79.728 31.405 71.412 1.00 35.07	С
ATOM	294 CD2 LEU A 345	80.562 33.373 72.617 1.00 35.91	С
ATOM	295 N LEUA 346	75.135 33.152 73.330 1.00 40.70	N
ATOM	296 CA LEU A 346	73.799 33.771 73.251 1.00 38.15	С
ATOM	297 C LEU A 346	73.411 34.515 74.514 1.00 37.81	С
ATOM	298 O LEU A 346	72.763 35.589 74.387 1.00 33.78	· O
ATOM	299 CB LEU A 346	72.812 32.717 72.775 1.00 36.63	С
ATOM	300 CG LEU A 346	73.197 32.163 71.396 1.00 36.54	С
ATOM	301 CD1 LEU A 346	72.319 30.952 71.093 1.00 39.38	С
ATOM	302 CD2 LEU A 346	73.117 33.221 70.327 1.00 34.92	С
ATOM	303 N THR A 347	73.767 34.006 75.697 1.00 35.86	N
ATOM	304 CA THR A 347	73.329 34.644 76.950 1.00 38.36	C
ATOM	305 C THR A 347	74.041 35.977 77.122 1.00 39.47	С
ATOM	306 O THR A 347	73.402 36.976 77.407 1.00 40.21	0
ATOM	307 CB THR A 347	73.610 33.797 78.194 1.00 38.11	С
ATOM	308 OG1 THR A 347	73.118 32.465 78.023 1.00 43.41	0
ATOM	309 CG2 THR A 347	73.043 34.344 79.455 1.00 32.94	С
ATOM	310 N ASN A 348	75.364 35.950 76.915 1.00 38.84	N
ATOM	311 CA ASN A 348	76.138 37.179 77.003 1.00 35.12	С
ATOM	312 C ASN A 348	75.528 38.199 76.057 1.00 31.75	C
ATOM	313 O ASN A 348	75.185 39.266 76.531 1.00 32.58	0
ATOM		77.627 36.954 76.674 1.00 39.35	C
ATOM		78.368 38.293 76.687 1.00 43.83	C
ATOM		78.520 38.958 75.647 1.00 47.22	0
ATOM		78.692 38.727 77.886 1.00 44.28	N
ATOM		75.332 37.861 74.793 1.00 29.26	N
ATOM		74.787 38.795 73.811 1.00 27.91	С
ATOM		73.486 39:418 74.289 1.00 31.58	C
ATOM		73.345 40.634 74.458 1.00 30.15	0
ATOM		74.719 38.088 72.472 1.00 28.75	C
ATOM		74.083 38.806 71.284 1.00 36.78	C
ATOM		74.865 40.076 70.945 1.00 36.43	C
ATOM		74.014 37.922 70.034 1.00 36.80	C
ATOM		72.447 38.621 74.572 1.00 32.99	N
ATOM	327 CA ALA A 350	71.158 39.047 75.016 1.00 32.50	С

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ATOM	328 C ALA A 350	71.244 40.028 76.184 1.00 34.81	С
ATOM	329 O ALA A 350	70.514 41.032 76.293 1.00 31.47	0
ATOM	330 CB ALA A 350	70.422 37.775 75.508 1.00 34.40	С
ATOM	331 N ASP A 351	72.157 39.696 77.119 1.00 35.11	N
ATOM	332 CA ASP A 351	72.290 40.545 78.304 1.00 36.10	С
ATOM	333 C ASP A 351	72.844 41.893 77.939 1.00 35.62	С
ATOM	334 O ASP A 351		Ο
ATOM	335 CB ASP A 351		С
ATOM	336 CG ASP A 351		С
ATOM	337 OD1 ASP A 351		0
ATOM	338 OD2 ASP A 351	73.077 37.876 80.611 1.00 50.85	0
ATOM	339 N ARG A 352		N
ATOM	340 CA ARG A 352		С
ATOM	341 C ARG A 352	73.280 43.905 75.885 1.00 32.48	С
ATOM	342 O ARG A 352		0
ATOM	343 CB ARG A 352		C
ATOM	344 CG ARG A 352		C
ATOM	345 CD ARG A 352		C
ATOM	346 NE ARG A 352		N
ATOM	347 CZ ARG A 352		С
ATOM	348 NH1 ARG A 352		N
ATOM	349 NH2 ARG A 352		N
ATOM	350 N GLU A 353	72.544 43.238 74.999 1.00 33.29	N
ATOM	351 CA GLU A 353		С
ATOM	352 C GLU A 353		С
ATOM	353 O GLU A 353	69.862 45.515 74.941 1.00 32.80	0
ATOM	354 CB GLU A 353		C
ATOM	355 CG GLU A 353		C
ATOM	356 CD GLU A 353		C
ATOM	357 OE1 GLU A 353		0
ATOM	358 OE2 GLU A 353		0
ATOM	359 N LEU A 354		N
ATOM	360 CA LEU A 354	69.120 44.156 77.132 1.00 33.42	С
ATOM	361 C LEU A 354	69.419 45.557 77.625 1.00 33.94	C.
ATOM	362 O LEU A 354	68.543 46.397 77.897 1.00 35.63	0
ATOM	363 CB LEU A 354	68.904 43.225 78.282 1.00 35.57	C
ATOM	364 CG LEU A 354		C
ATOM	365 CD1 LEU A 354		C
ATOM	366 CD2 LEU A 354		C
ATOM	367 N VAL A 355	70.709 45.904 77.740 1.00 34.11	N
ATOM	368 CA VAL A 355	71.022 47.248 78.253 1.00 29.81	C
ATOM	369 C VAL A 355	70.578 48.281 77.275 1.00 32.35	C
ATOM	370 O VAL A 355	70.082 49.363 77.548 1.00 32.21	o
ATOM	371 CB VAL A 355		C
ATOM	372 CG1 VAL A 355		C
ATOM	373 CG2 VAL A 355		C
ATOM	374 N HIS A 356	70.801 48.019 75.969 1.00 35.17	N
ATOM	375 CA HIS A 356	70.469 49.090 75.019 1.00 34.30	C
ATOM	376 C HIS A 356	68.976 49.210 74.878 1.00 37.61	С

ATOM	377 O HIS A 356		0
ATOM	378 CB HIS A 356	71.119 48.696 73.700 1.00 37.14	С
ATOM	379 CG HIS A 356	72.604 48.940 73.811 1.00 40.21	С
ATOM	380 ND1 HIS A 356	73.150 50.199 73.687 1.00 40.55	N
ATOM	381 CD2 HIS A 356	73.615 48.091 74.046 1.00 41.21	С
ATOM	382 CE1 HIS A 356	74.457 50.080 73.844 1.00 42. 06	C
ATOM	383 NE2 HIS A 356	74.762 48.822 74.038 1.00 41.48	N
ATOM	384 N MET A 357	68.298 48.067 75.070 1.00 34.83	N
ATOM	385 CA MET A 357	66.873 48.010 74.942 1.00 34.72	С
ATOM	386 C MET A 357	66.214 48.979 75.895 1.00 39.56	С
ATOM	387 O MET A 357	65,178 49.613 75.547 1.00 41.07	0
ATOM	388 CB MET A 357	66.368 46.576 75.232 1.00 35.23	С
ATOM	389 CG MET A 357	64.941 46.399 74.752 1.00 32.18	С
ATOM	390 SD MET A 357	64.275 44.817 75.326 1.00 34.77	S
ATOM	391 CE MET A 357	65.449 43.688 74.619 1.00 34.80	С
ATOM	392 N ILE A 358	66,795 49,034 77,102 1,00 38,12	N
ATOM	393 CA ILE A 358	66.256 49.963 78.081 1.00 40.67	С
ATOM	394 C ILE A 358	66.347 51.379 77.587 1.00 44.25	С
ATOM	395 O ILE A 358	65.338 52.129 77.678 1.00 48.55	0
ATOM	396 CB ILE A 358	66.916 49.765 79.451 1.00 40.93	С
ATOM	397 CG1 ILE A 358	66,228 48.488 80.022 1.00 39.31	С
ATOM	398 CG2 ILE A 358	66.637 50.945 80.347 1.00 39.18	С
ATOM	399 CD1 ILE A 358	67.075 47.683 80.909 1.00 39.58	С
ATOM	400 N ASN A 359	67.514 51.758 77.039 1.00 40.76	N
ATOM	401 CA ASN A 359	67.626 53.090 76.513 1.00 40.91	С
ATOM	402 C ASN A 359	66.563 53.275 75.414 1.00 39.09	С
ATOM	403 O ASN A 359	66.079 54.381 75.223 1.00 42.57	0
ATOM	404 CB ASN A 359	68.936 53.472 75.833 1.00 44.08	С
ATOM	405 CG ASN A 359	70.118 53.378 76.729 1.00 51.07	С
ATOM	406 OD1 ASN A 359	69.922 53.474 77.967 1.00 55.22	0
ATOM	407 ND2 ASN A 359	71.312 53.183 76.144 1.00 50.95	N
ATOM	408 N TRP A 360	66.430 52.328 74.532 1.00 36.27	N
ATOM	409 CA TRP A 360	65.485 52.489 73.414 1.00 36.80	С
ATOM	410 C TRP A 360	64.084 52.609 73.992 1.00 40.32	С
ATOM	411 O TRP A 360	63.265 53.514 73.773 1.00 37.53	Ο
ATOM		65.706 51.293 72.489 1.00 32.87	С
ATOM		64.495 51.101 71.623 1.00 36.76	C
ATOM		64.249 51.724 70.450 1.00 35.10	С
ATOM		63.406 50.191 71.847 1.00 36.41	С
ATOM		63.093 51.271 69.921 1.00 35.72	N
ATOM		62.517 50.381 70.778 1.00 38.84	С
ATOM	. –	63.083 49.270 72.848 1.00 35.46	С
ATOM		61.270 49.707 70.703 1.00 40.31	С
ATOM		61.888 48.580 72.776 1.00 35.51	C
ATOM		61.007 48.822 71.707 1.00 39.13	C
ATOM		63.731 51.677 74.909 1.00 40.42	N
ATOM		62.394 51.784 75.480 1.00 43.31	C
ATOM		62.074 53.205 75.921 1.00 43.29	C
ATOM		60.935 53.682 75.778 1.00 40.16	Ō
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ATOM	426 CB ALA A 361	62.223 50.861 76.695 1.00 44:40	С
ATOM	427 N LYS A 362		N
ATOM	428 CA LYS A 362	62.873 55.140 77.180 1.00 44.02	C
ATOM	429 C LYS A 362	62.644 56.183 76.120 1.00 44.20	С
ATOM	430 O LYS A 362	62.172 57.257 76.432 1.00 46.12	Ο
ATOM	431 CB LYS A 362	64.028 55.467 78.102 1.00 45.07	С
ATOM	432 CG LYS A 362	64.099 54.601 79.360 1.00 45.39	С
ATOM	433 CD LYS A 362	63.760 55,450 80.584 1.00 50.39	С
ATOM	434 CE LYS A 362	63.073 54.690 81.677 1.00 54.46	С
ATOM	435 NZ LYS A 362	62.697 55.356 82.942 1.00 53.54	N
ATOM	436 N ARG A 363	62.896 55.918 74.859 1.00 46.04	N
ATOM	437 CA ARG A 363	62.666 56.783 73.735 1.00 48.68	С
ATOM	438 C ARG A 363	61.350 56.466 72.999 1.00 49.08	C
ATOM	439 O ARG A 363	60.941 57.054 71.977 1.00 48.73	0
ATOM	440 CB ARG A 363	63.836 56.643 72.757 1.00 53.32	C
ATOM	441 CG ARG A 363	64.902 57.723 72.904 1.00 60.34	C
ATOM	442 CD ARG A 363		С
ATOM	443 NE ARG A 363		. N
ATOM	444 CZ ARG A 363		С
ATOM	445 NH1 ARG A 363		N
ATOM	446 NH2 ARG A 363	69.002 58.051 75.459 1.00 84.83	N
ATOM	447 N VAL A 364	60.623 55.453 73.448 1.00 45.49	N
ATOM	448 CA VAL A 364		C
ATOM	449 C VAL A 364		C
ATOM	450 O VAL A 364	57.817 55.984 74.385 1.00 55.07	0
ATOM	451 CB VAL A 364		C
ATOM	452 CG1 VAL A 364		C
ATOM	453 CG2 VAL A 364		C
ATOM	454 N PRO A 365	57.746 56.755 72.334 1.00 56.52	N
ATOM	455 CA PRO A 365		C
ATOM	456 C PRO A 365		С
ATOM	457 O PRO A 365		0
ATOM	458 CB PRO A 365	56.078 58.059 71.257 1.00 56.19	C
ATOM	459 CG PRO A 365	57.446 58.203 70.542 1.00 58.84	C
ATOM	460 CD PRO A 365	58.160 56.882 70.922 1.00 58.70	N
ATOM	461 N GLY A 366		C
ATOM	462 CA GLY A 366	54.426 57.130 75.628 1.00 56.39	C
ATOM	463 C GLY A 366	55.063 56.367 76.771 1.00 56.65	0
ATOM	464 O GLY A 366	54.553 56.398 77.893 1.00 56.35	N
ATOM	465 N PHE A 367	56.197 55.701 76.480 1.00 54.46	C
ATOM	466 CA PHE A 367	56.848 54.870 77.461 1.00 49.74	C
ATOM	467 C PHE A 367	57.198 55.574 78.738 1.00 49.68	0
ATOM	468 O PHE A 367	56.884 55.121 79.814 1.00 51.83	C
ATOM	469 CB PHE A 367	58.152 54.252 76.951 1.00 46.86 58.531 53.053 77.781 1.00 43.25	C
ATOM	470 CG PHE A 367	58.531 53.053 77.781 1.00 43.25	C
ATOM	471 CD1 PHE A 367	57.785 51.876 77.698 1.00 42.05 59.593 53.110 78.639 1.00 40.49	C
ATOM	472 CD2 PHE A 367		C
ATOM	473 CE1 PHE A 367		C
ATOM	474 CE2 PHE A 367	59.962 51.999 79.388 1.00 41.57	C

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ATOM		59.241 50.822 79.270 1.00 41.29	C
ATOM	476 N VAL A 368		N
ATOM	477 CA VAL A 368	58.277 57.398 79.845 1.00 55.10	C
ATOM	478 C VAL A 368	57.222 58.255 80.487 1.00 57.40	C
ATOM	479 O VAL A 368	57.476 58.969 81.463 1.00 60.79	0
ATOM	480 CB VAL A 368		C
ATOM	481 CG1 VAL A 368		C
ATOM	482 CG2 VAL A 368		C
ATOM	483 N ASP A 369	55.977 58.178 80.074 1.00 59.67	N
ATOM	484 CA ASP A 369	54.828 58.794 80.705 1.00 60.47	С
ATOM	485 C ASP A 369		C
ATOM	486 O ASP A 369		0
ATOM	487 CB ASP A 369		C
ATOM	488 CG ASP A 369	54.038 60.056 78.677 1.00 67.29	C
ATOM	489 OD1 ASP A 369	54.913 60.914 78.918 1.00 72.50	0
ATOM	490 OD2 ASP A 369		0
ATOM	491 N LEU A 370		N
ATOM	492 CA LEU A 370	54.194 55.517 82.497 1.00 56.12	C
ATOM	493 C LEU A 370	55.117 55.633 83.719 1.00 57.05	C
ATOM	494 O LEU A 370		0
ATOM	495 CB LEU A 370	54.224 54.086 82.012 1.00 53.92	C
ATOM	496 CG LEU A 370	53.750 53.771 80.597 1.00 51.91	C
ATOM	497 CD1 LEU A 370	54.145 52.344 80.254 1.00 49.81	C
ATOM	498 CD2 LEU A 370		C
ATOM	499 N THR A 371		N
ATOM	500 CA THR A 371	55.305 54.930 86.062 1.00 54.21	C
ATOM	501 C THR A 371		C
ATOM	502 O THR A 371		0
ATOM	503 CB THR A 371		C
ATOM		53.969 53.073 86.858 1.00 51.61	O C
ATOM	505 CG2 THR A 371		
ATOM		57.455 53.969 86.615 1.00 57.36	N
ATOM	507 CA LEU A 372	58.566 53.062 86.620 1.00 58.29	C
ATOM	508 C LEU A 372	58.120 51.623 86.694 1.00 60.17	C
ATOM	509 O LEU A 372	58.503 50.771 85.878 1.00 63.49	0
ATOM		59.497 53.427 87.759 1.00 57.98	C C
ATOM		60.669 52.498 88.043 1.00 59.29	C
ATOM	512 CD1 LEU A 372	61.657 52.449 86.860 1.00 56.28	C
ATOM	513 CD2 LEU A 372	61.371 52.966 89.312 1.00 58.46	N
ATOM		57.266 51.300 87.638 1.00 63.16	C
ATOM		56.736 49.927 87.758 1.00 65.55	c
ATOM		55.954 49.441 86.539 1.00 57.99	Ö
ATOM	517 O HIS A 373	56.039 48.257 86.199 1.00 54.67	C
ATOM		55.946 49.829 89.074 1.00 69.47	C
ATOM		54.720 49.000 88.987 0.50 73.73	C
ATOM	520 CG BHIS A 373	56.788 50.250 90.240 0.50 73.05	N
ATOM	521 ND1AHIS A 373		N
ATOM			C
ATOM	523 CD2AHIS A 373	54.497 47.674 89.164 0.50 74.74	C

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ATOM	524 CD2BHIS A 373	56.824 51.436 90.897 0.50 73.60	С
ATOM	525 CE1AHIS A 373	52.587 48.602 88.589 0.50 76.98	С
ATOM	526 CE1BHIS A 373	58.323 50.101 91.800 0.50 74.02	С
ATOM	527 NE2AHIS A 373	53.168 47.451 88.911 0.50 75.88	N
ATOM	528 NE2BHIS A 373	57.785 51.306 91.873 0.50 74.59	N
ATOM		55.238 50.282 85.826 1.00 51.93	N
ATOM		54.551 49.869 84.597 1.00 51.38	С
ATOM		55.515 49.657 83.442 1.00 48.48	С
ATOM		55.319 48.767 82.638 1.00 44.30	0
ATOM		53.450 50.853 84.249 1.00 50.24	С
ATOM	534 CG ASP A 374	52,230 50,420 85,062 1,00 52,68	С
ATOM	535 OD1 ASP A 374	52.218 49.208 85.463 1.00 51.70	0
ATOM	536 OD2 ASP A 374	51.373 51.283 85.253 1.00 53.06	0
ATOM	537 N GLN A 375	56.573 50.488 83.455 1.00 45.36	N
ATOM	538 CA GLN A 375	57.656 50.360 82.495 1.00 41.61	С
ATOM	539 C GLN A 375	58,283 48,993 82,695 1,00 39,41	С
ATOM	540 O GLN A 375	58.336 48.206 81.773 1.00 41.05	0
ATOM	541 CB GLN A 375	58.722 51.381 82.876 1.00 41.76	С
ATOM	542 CG GLN A 375	58.141 52.753 82.526 1.00 45.94	С
ATOM	543 CD GLN A 375	59.172 53.861 82.496 1.00 43.23	С
ATOM	544 OE1 GLN A 375	60.348 53.687 82.769 1.00 43.50	0
ATOM	545 NE2 GLN A 375	58.662 55.017 82.109 1.00 42.26	N
ATOM	546 N VAL A 376	58.641 48.685 83.938 1.00 36.73	N.
ATOM	547 CA VAL A 376	59.196 47.368 84.224 1.00 37.97	С
ATOM	548 C VAL A 376	58.282 46.277 83.719 1.00 41.67	С
ATOM	549 O VAL A 376	58.716 45.290 83.122 1.00 45.19	Ο
ATOM	550 CB VAL A 376	59.469 47.195 85.731 1.00 35.47	С
ATOM	551 CG1 VAL A 376	59.965 45.806 86.083 1.00 30.36	С
ATOM	552 CG2 VAL A 376	60.478 48.183 86.231 1.00 33.53	С
ATOM		56.969 46.410 83.927 1.00 44.51	N
ATOM			С
ATOM		56.050 45.247 81.960 1.00 42.12	C
ATOM		56.204 44.128 81.478 1.00 40.13	0
ATOM	557 CB HIS A 377	54.614 45.523 84.024 1.00 55.12	C
ATOM	558 CG AHIS A 377	54.584 45.136 85.476 0.50 58.91	C
ATOM	559 CG BHIS A 377	53.722 44.380 83.605 0.50 62.01	C
ATOM	560 ND1AHIS A 377	54.578 46.053 86.503 0.50 62.18	N
ATOM	561 ND1BHIS A 377	52.391 44.275 83.949 0.50 63.95	N
ATOM	562 CD2AHIS A 377	54.630 43.920 86.064 0.50 60.71	C
ATOM	563 CD2BHIS A 377	53.959 43.265 82.854 0.50 65.09	C
ATOM	564 CE1AHIS A 377	54.592 45.421 87.664 0.50 63.07	C
ATOM	565 CE1BHIS A 377	51.870 43.175 83.442 0.50 64.35	C
ATOM	566 NE2AHIS A 377	54.617 44.116 87.425 0.50 62.25	N
ATOM	567 NE2BHIS A 377	52.805 42.538 82.765 0.50 65.59	N
ATOM	568 N LEU A 378	55.875 46.306 81.194 1.00 40.05	N
ATOM	569 CA LEU A 378	56.069 46.198 79.753 1.00 37.29	C
ATOM	570 C LEU A 378	57.391 45.520 79.441 1.00 38.78	C
ATOM	571 O LEU A 378	57.419 44.461 78.742 1.00 36.97	0
ATOM	572 CB LEU A 378	55.891 47.583 79.166 1.00 35.55	С

C 54.472 48.193 79.308 1.00 35.81 573 CG LEU A 378 ATOM C 574 CD1 LEU A 378 54.392 49.470 78.484 1.00 30.30 **ATOM** C 53,362 47.280 78.812 1.00 31.78 575 CD2 LEU A 378 **ATOM** N 58.553 45.941 79.947 1.00 37.44 576 N LEU A 379 **ATOM** 59.758 45.222 79.522 1.00 38.20 C 577 CA LEU A 379 ATOM 59,791 43,802 79,976 1.00 37,44 C 578 C LEU A 379 ATOM 60.111 42.892 79.212 1.00 40.19 0 579 O LEU A 379 ATOM 61.058 45.907 79.913 1.00 39.04 C 580 CB LEU A 379 **ATOM** C 61,325 47,100 79,006 1,00 39,22 581 CG LEU A 379 ATOM C 62.112 48.158 79.710 1.00 42.38 582 CD1 LEU A 379 ATOM C 62.004 46.589 77.765 1.00 41.99 583 CD2 LEU A 379 ATOM 584 N GLU A 380 59.450 43.551 81.214 1.00 40.36 N ATOM 585 CA GLU A 380 59.453 42.181 81.682 1.00 41.72 C ATOM C 58.810 41.256 80.662 1.00 43.73 586 C GLU A 380 ATOM 587 O GLU A 380 0 59.412 40.219 80.382 1.00 44.30 ATOM 58.749 42.072 83.019 1.00 44.70 C 588 CB GLU A 380 ATOM C 59,462 40,967 83,836 1,00 54,40 589 CG GLU A 380 ATOM 58.603 40.469 84.968 1.00 59.95 C 590 CD GLU A 380 ATOM 0 57.640 41.190 85.359 1.00 64.57 591 OE1 GLU A 380 ATOM 0 58.858 39.364 85.491 1.00 62.18 ATOM 592 OE2 GLU A 380 57.620 41.585 80.171 1.00 40.13 N 593 N CYS A 381 ATOM C 594 CA CYS A 381 56.913 40.781 79.214 1.00 43.11 ATOM 57.398 40.814 77.770 1.00 41.34 C 595 C CYS A 381 **ATOM** 57.371 39.795 77.080 1.00 37.54 0 596 O CYS A 381 ATOM 55,444 41,227 79,248 1,00 51,91 C 597 CB CYS A 381 ATOM S 54.415 40.723 80.635 0.50 58.51 598 SG ACYS A 381 ATOM ·S 54,457 40.510 80.604 0.50 56.75 599 SG BCYS A 381 **ATOM** 600 N ALA A 382 57.838 41.858 77.157 1.00 38.84 N ATOM C 58.257 42.011 75.817 1.00 40.08 601 CA ALA A 382 ATOM 59.715 41.782 75.473 1.00 40.25 C 602 C ALA A 382 ATOM 59.985 41.601 74.285 1.00 38.99 0 603 O ALA A 382 ATOM 58.042 43.529 75.430 1.00 39.43 C 604 CB ALA A 382 ATOM 60.614 41.752 76.463 1.00 39.37 N 605 N TRP A 383 ATOM C 62.029 41.668 76.112 1.00 34.09 606 CA TRP A 383 ATOM 62.359 40.622 75.103 1.00 31.78 C 607 C TRP A 383 ATOM 63.015 40.905 74.096 1.00 32.20 0 608 O TRP A 383 ATOM 62.859 41.672 77.383 1.00 35.92 C 609 CB TRP A 383 ATOM C 62.819 40.332 78.083 1.00 36.18 610 CG TRP A 383 ATOM C 61.988 39.877 79.045 1.00 33.74 611 CD1 TRP A 383 ATOM C 63.738 39.252 77.793 1.00 32.73 612 CD2 TRP A 383 ATOM 62.314 38.588 79.374 1.00 31.23 N 613 NE1 TRP A 383 ATOM C 63.379 38.189 78.617 1.00 31.78 614 CE2 TRP A 383 ATOM C 64.791 39.129 76.910 1.00 33.23 615 CE3 TRP A 383 ATOM C 64.065 36.985 78.590 1.00 34.54 616 CZ2 TRP A 383 ATOM C 617 CZ3 TRP A 383 65.487 37.948 76.872 1.00 37.35 **ATOM** C 65.114 36.888 77.709 1.00 39.46 ATOM 618 CH2 TRP A 383

61.904 39.399 75.220 1.00 32.57

61.644 38.543 72.923 1.00 33.24

62.253 38.338 74.291 1.00 31.20

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ATOM

ATOM

ATOM

619 N LEU A 384

620 CA LEU A 384

621 C LEU A 384

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ATOM	622 O LEU A 384	62.338 38.321 71.921 1.00 36.36	Ο
ATOM	623 CB LEU A 384	61.901 36.984 74.846 1.00 30.65	С
ATOM	624 CG LEU A 384	62.520 35.799 74.124 1.00 34.98	С
ATOM	625 CD1 LEU A 384	4 64.011 35.983 73.843 1.00 36.19	С
ATOM	626 CD2 LEU A 384	4 62.277 34.525 74.920 1.00 33.80	С
ATOM	627 N GLU A 385	60.426 39.016 72.851 1.00 31.93	N
ATOM	628 CA GLU A 385	5 59,761 39,353 71,602 1.00 33.94	С
ATOM	629 C GLU A 385	60.602 40.397 70.858 1.00 32.22	С
ATOM	630 O GLU A 385	60.817 40.376 69.660 1.00 33.72	0
ATOM	631 CB GLU A 385	5 58.370 39.960 71.823 1.00 35.67	С
ATOM	632 CG GLU A 385	5 57.399 39.108 72.631 1.00 38.33	С
ATOM	633 CD GLU A 385	55.994 39.641 72.528 1.00 40.58	С
ATOM	634 OE1 GLU A 38	5 55.547 39.798 71.400 1.00 40.46	O
ATOM	635 OE2 GLU A 38	5 55.290 39.935 73.508 1.00 46.27	O
ATOM	636 N ILE A 386	61.074 41.363 71.631 1.00 33.24	N
ATOM	637 CA ILE A 386	61.890 42.428 71.095 1.00 34.08	С
ATOM	638 C ILE A 386	63.252 41.946 70.640 1.00 32.42	С
ATOM	639 O ILE A 386	63.662 42.262 69.535 1.00 30.26	О
ATOM	640 CB ILE A 386	61.988 43.548 72.115 1.00 36.86	С
ATOM	641 CG1 ILE A 386	60.540 44.052 72.312 1.00 34.58	С
ATOM	642 CG2 ILE A 386	62.928 44.623 71.558 1.00 34.85	С
ATOM	643 CD1 ILE A 386	60.405 45.082 73.399 1.00 35.95	С
ATOM	644 N LEU A 387	63.928 41.081 71.387 1.00 28.96	N.
ATOM	645 CA LEU A 387	65.174 40.562 70.881 1.00 29.61	С
ATOM	646 C LEU A 387	64.858 39.779 69.603 1.00 32.09	С
ATOM	647 O LEU A 387	65.705 39.742 68.698 1.00 34.46	О
ATOM	648 CB LEU A 387	65.889 39.569 71.835 1.00 27.75	С
ATOM	649 CG LEU A 387	66.424 40.175 73.143 1.00 26.77	С
ATOM	650 CD1 LEU A 38	7 67.288 39.131 73.866 1.00 23.67	С
ATOM	651 CD2 LEU A 38	7 67.178 41.469 72.900 1.00 20.60	С
ATOM	652 N MET A 388	63.715 39.109 69.599 1.00 31.37	N
ATOM	653 CA MET A 388	8 63.407 38.271 68.455 1.00 32.11	С
ATOM	654 C MET A 388	63.050 39.074 67.251 1.00 34.52	С
ATOM	655 O MET A 388	63.618 38.897 66.152 1.00 39.16	0
ATOM	656 CB MET A 388	8 62.369 37.292 68.899 1.00 35.14	C
ATOM	657 CG MET A 38	8 62.997 36.132 69.696 1.00 34.54	С
ATOM	658 SD MET A 388	8 61.579 35.037 70.144 1.00 31.08	S
ATOM	659 CE MET A 388	8 62.630 33.726 70.818 1.00 28.15	С
ATOM	660 N ILE A 389	62.163 40.064 67.378 1.00 31.76	N
ATOM	661 CA ILE A 389	61.937 40.845 66.157 1.00 28.08	С
ATOM	662 C ILE A 389	63.220 41.450 65.674 1.00 27.99	С
ATOM	663 O ILE A 389	63.340 41.443 64.445 1.00 33.28	О
ATOM	664 CB ILE A 389	60.741 41.789 66.277 1.00 29.02	С
ATOM	665 CG1 ILE A 389		С
ATOM	666 CG2 ILE A 389		С
ATOM	667 CD1 ILE A 389		С
ATOM	668 N GLY A 390	64.202 41.873 66.409 1.00 31.34	N
ATOM	669 CA GLY A 390	65.489 42.435 65.959 1.00 32.81	С
ATOM	670 C GLY A 390	66.289 41.365 65.202 1.00 37.06	С

ATOM	671 O GLY A 390	66.893 41.578 64.121 1.00 34.61	0
ATOM		66.214 40.147 65.760 1.00 36.24	N
ATOM		66.917 39.020 65.149 1.00 37.58	С
ATOM		66.366 38.746 63.762 1.00 38.13	С
ATOM		66.998 38.644 62.734 1.00 41.32	0
ATOM		66.696 37.733 65.989 1.00 34.64	С
ATOM	677 CG LEU A 391	67.358 36.473 65.437 1.00 34.89	С
ATOM	678 CD1 LEU A 391	68.884 36.663 65.425 1.00 32.05	С
ATOM	679 CD2 LEU A 391	67.013 35.204 66.176 1.00 30.69	С
ATOM	680 N VAL A 392		N
ATOM		64.396 38.272 62.452 1.00 35.17	С
ATOM	682 C VAL A 392	64.699 39.339 61.446 1.00 36.85	С
ATOM		65.135 39.107 60.309 1.00 35.69	0
ATOM	684 CB VAL A 392	62.905 38.051 62.725 1.00 31.86	С
ATOM		62.145 38.115 61.450 1.00 33.20	С
ATOM		62.744 36.672 63.376 1.00 29.17	С
ATOM		64.502 40.589 61.879 1.00 38.90	N
ATOM		64.798 41.685 60.919 1.00 40.63	С
ATOM		66.238 41.713 60.430 1.00 41.64	С
ATOM		66.577 41.830 59.234 1.00 42.66	0
ATOM		64.334 42.968 61.524 1.00 36.63	С
ATOM		64.978 44.145 60.878 1.00 41.40	С
ATOM		66.133 44.745 61.230 1.00 42.92	С
ATOM		64.442 44.911 59.802 1.00 44.52	С
ATOM		66.348 45.849 60.435 1.00 43.05	N
ATOM	696 CE2 TRP A 393	65.340 45.971 59.552 1.00 44.85	С
ATOM	697 CE3 TRP A 393	63.273 44.834 59.038 1.00 46.64	C
ATOM	698 CZ2 TRP A 393	65.125 46.909 58.530 1.00 47.52	C
ATOM		63.050 45.763 58.042 1.00 46.72	C
ATOM		63.976 46.788 57.787 1.00 46.56	С
ATOM			N
ATOM		68.609 41.594 60.787 1.00 38.26	С
ATOM		69.005 40.350 60.060 1.00 40.13	C
ATOM	704 O ARG A 394	70.050 40.371 59.402 1.00 44.10	0
ATOM	_	69.669 42.039 61.742 1.00 36.59	C
ATOM		70.204 41.076 62.746 1.00 34.20	C C
ATOM		70.465 41.819 64.103 1.00 28.97	N
ATOM		70.926 40.678 65.024 1.00 28.34	C
ATOM		70.320 40.727 66.245 1.00 27.62	
ATOM		69.464 41.713 66.453 1.00 19.82	N N
ATOM		70.587 39.885 67.213 1.00 25.67	N
ATOM		68.208 39.318 60.111 1.00 41.76	C
ATOM		68.452 38.051 59.429 1.00 38.35	c
ATOM		67.806 38.064 58.044 1.00 42.96	0
ATOM		68.042 37.142 57.249 1.00 43.79 67.787 36.988 60.304 1.00 33.00	C
ATOM		68.581 36.712 61.393 1.00 32.59	o
ATOM		66.920 39.018 57.733 1.00 46.08	N
ATOM		66.241 39.028 56.474 1.00 52.16	C
ATOM	719 CA MET A 396	00.241 39.028 30.474 1.00 32.10	

		(8 000 00 810 55 045 1 00 55 80	_
ATOM	720 C MET A 396		C
ATOM		66.630 38.021 54.347 1.00 58.39	0
ATOM	722 CB MET A 396	65.692 40.431 56.132 1.00 52.31	C
ATOM	723 CG MET A 396	64.582 40.764 57.105 1.00 56.91	C
ATOM	724 SD MET A 396	63.629 42.054 56.328 1.00 63.07	S
ATOM	725 CE MET A 396	64.823 43.416 56.452 1.00 64.89	C
ATOM	726 N GLU A 397	68.248 39.308 55.134 1.00 60.31	N
ATOM	727 CA GLU A 397		С
ATOM	728 C GLU A 397	70.057 37.952 54.074 1.00 65.23	С
ATOM	729 O GLU A 3 97	71.096 37.919 53.392 1.00 67.51	О
ATOM	730 CB GLU A 397	69.836 40.417 53.676 1.00 63.51	С
ATOM	731 CG GLU A 397	68.932 41.412 52.969 1.00 63.47	С
ATOM	735 N HIS A 398	69.810 36.962 54.918 1.00 62.92	N
ATOM	736 CA HIS A 398	70.655 35.813 55.141 1.00 61.99	С
ATOM	737 C HIS A 398	69.769 34.568 55.190 1.00 63.69	С
ATOM	738 O HIS A 398	69.650 33.874 56.210 1.00 64.15	0
ATOM	739 CB HIS A 398	71.494 35.908 56.435 1.00 60.76	С
ATOM	740 CG HIS A 398	72.350 37.130 56.441 1.00 62.00	С
ATOM	741 ND1 HIS A 398	73.602 37.138 55.871 1.00 62.89	N
ATOM	742 CD2 HIS A 398	72.159 38.382 56.907 1.00 63.78	С
ATOM	743 CE1 HIS A 398	74.136 38.343 55.996 1.00 63.12	С
ATOM	744 NE2 HIS A 398	73.287 39.130 56.626 1.00 63.82	N
ATOM	745 N PRO A 399	69.118 34.298 54.072 1.00 64.36	N.
ATOM	746 CA PRO A 399	68.245 33.161 53.880 1.00 63.44	С
ATOM	747 C PRO A 399	68.777 31.873 54.445 1.00 62.06	С
ATOM	748 O PRO A 399	69.878 31.459 54.055 1.00 66.41	O
ATOM	749 CB PRO A 399	68.065 32.967 52.358 1.00 66.29	С
ATOM	750 CG PRO A 399	68.811 34.124 51.755 1.00 67.27	Ċ
ATOM	751 CD PRO A 399		Ċ
ATOM	752 N GLY A 400	68.081 31.209 55.340 1.00 59.48	N
ATOM	753 CA GLY A 400	68.581 29.943 55.883 1.00 58.66	C
ATOM	754 C GLY A 400	69.420 30.084 57.129 1.00 59.22	C
ATOM	755 O GLY A 400	69.649 29.125 57.892 1.00 57.75	ŏ
ATOM	756 N LYS A 401	69.779 31.333 57.419 1.00 60.49	N
ATOM	757 CA LYS A 401	70.647 31.575 58.580 1.00 61.65	C
ATOM		70.064 32.683 59.437 1.00 59.45	c
ATOM		69.238 33.473 58.937 1.00 60.63	ŏ
ATOM		71.995 31.976 57.973 1.00 67.13	C
ATOM		72.926 30.812 57.630 1.00 72.43	Č
ATOM	762 CD LYS A 401	74.002 31.223 56.630 1.00 75.81	Č
ATOM		74.975 30.083 56.376 1.00 78.81	Č
		76.395 30.528 56.184 1.00 80.22	N
ATOM			N
ATOM		70.423 32.708 60.711 1.00 52.61	C
ATOM	766 CA LEU A 402	70.066 33.765 61.639 1.00 45.10	
ATOM		71.344 34.513 62.075 1.00 43.73	C
ATOM		72.298 33.996 62.654 1.00 39.37	0
ATOM		69.399 33.237 62.909 1.00 42.38	C
ATOM		68.120 32.435 62.728 1.00 39.82	C
ATOM	771 CD1 LEU A 402	67.769 31.650 63.986 1.00 39.53	C

66.993 33.374 62.319 1.00 39.35 C 772 CD2 LEU A 402 ATOM N 71.300 35.810 61.904 1.00 42.24 773 N LEU A 403 **ATOM** C 72.268 36.780 62.299 1.00 40.59 774 CA LEU A 403 ATOM 72.049 37.247 63.735 1.00 41.66 C 775 C LEU A 403 **ATOM** 0 71.713 38.394 64.144 1.00 41.67 776 O LEU A 403 ATOM 72.238 37.958 61.311 1.00 42.13 C 777 CB LEU A 403 ATOM C 73.447 38.895 61.429 1.00 46.14 778 CG LEU A 403 ATOM C 74.639 38.172 60.823 1.00 49.15 779 CD1 LEU A 403 ATOM C 73.227 40.203 60.714 1.00 49.49 780 CD2 LEU A 403 ATOM 72.408 36.321 64.654 1.00 40.36 N 781 N PHE A 404 **ATOM** 72.406 36.715 66.070 1.00 41.94 C 782 CA PHE A 404 **ATOM** 73.318 37.929 66.247 1.00 41.94 C 783 C PHE A 404 **ATOM** 72.974 38.820 66.991 1.00 42.90 0 784 O PHE A 404 **ATOM** 72.843 35.598 66.931 1.00 42.78 C 785 CB PHE A 404 **ATOM** C 71.768 34.592 67.146 1.00 43.78 786 CG PHE A 404 **ATOM** C 70.810 34.769 68.112 1.00 44.40 787 CD1 PHE A 404 **ATOM** 71.748 33.445 66.381 1.00 46.28 C 788 CD2 PHE A 404 ATOM C 69.841 33.791 68.313 1.00 43.91 789 CE1 PHE A 404 ATOM 70.771 32.465 66.574 1.00 44.73 C 790 CE2 PHE A 404 **ATOM** 69.833 32.653 67.543 1.00 43.94 C 791 CZ PHE A 404 **ATOM** 74,436 37,946 65,571 1.00 42,52 N 792 N ALA A 405 **ATOM** 75.370 39.061 65.568 1.00 42.15 C 793 CA ALA A 405 ATOM 76.167 38.912 64.249 1.00 43.61 C 794 C ALA A 405 **ATOM** 76.106 37.832 63.651 1.00 45.81 0 795 O ALA A 405 ATOM 76.301 39.170 66.715 1.00 39.38 C 796 CB ALA A 405 **ATOM** 76.861 39.956 63.875 1.00 40.72 N 797 N PRO A 406 **ATOM** C 77.624 39.995 62.645 1.00 40.43 798 CA PRO A 406 **ATOM** C 78.662 38.899 62.665 1.00 44.15 799 C PRO A 406 **ATOM** 78.908 38.153 61.706 1.00 46.52 0 800 O PRO A 406 **ATOM** 78.192 41.408 62.548 1.00 39.43 C 801 CB PRO A 406 ATOM 77,309 42,186 63,509 1.00 38,57 C 802 CG PRO A 406 ATOM 76.899 41.234 64.592 1.00 38.37 C 803 CD PRO A 406 **ATOM** 79.299 38.719 63.824 1.00 45.92 N 804 N ASN A 407 **ATOM** 80.292 37.685 63.991 1.00 47.14 C 805 CA ASN A 407 **ATOM** C 79.688 36.384 64.518 1.00 47.74 806 C ASN A 407 **ATOM** 80.540 35.607 64.997 1.00 49.51 0 807 O ASN A 407 **ATOM** 81.401 38.056 64.970 1.00 49.67 C 808 CB ASN A 407 ATOM 80.967 38.449 66.364 1.00 48.87 809 CG ASN A 407 ATOM 0 79.848 38.858 66.629 1.00 47.25 810 OD1 ASN A 407 ATOM N 81,904 38,361 67,311 1,00 46,89 811 ND2 ASN A 407 ATOM 78.395 36.163 64.444 1.00 43.98 N 812 N LEU A 408 **ATOM** 77.840 34.907 64.942 1.00 44.28 C 813 CA LEU A 408 ATOM C 76.574 34.578 64.137 1.00 48.56 814 C LEU A 408 ATOM 75.483 34.720 64.657 1.00 50.61 O 815 O LEU A 408 ATOM 77.399 35.004 66.412 1.00 41.78 C 816 CB LEU A 408 ATOM C 76.965 33.709 67.060 1.00 37.59 817 CG LEU A 408 ATOM 77.962 32.592 66.735 1.00 42.03 C 818 CD1 LEU A 408 ATOM C 76.774 33.777 68.536 1.00 37.24 819 CD2 LEU A 408 ATOM 76.739 34.248 62.895 1.00 50.15 N 820 N LEU A 409 ATOM

ATOM	821 CA LEU A 409	75.691 33.915 61.969 1.00 53.65	С
ATOM	822 C LEU A 409	75.440 32.418 61.915 1.00 55.29	С
ATOM	823 O LEU A 409	76.158 31.729 61.190 1.00 59.32	O
ATOM	824 CB LEU A 409	76.154 34.481 60.614 1.00 52.50	С
ATOM	825 CG LEU A 409	75.026 34.637 59.601 1.00 54.30	С
ATOM	826 CD1 LEU A 409	75.459 35.371 58.345 1.00 54.05	С
	827 CD2 LEU A 409	74.550 33.227 59.271 1.00 53.81	С
ATOM	S28 N LEU A 410	74.481 31.871 62.624 1.00 55.42	N
ATOM	829 CA LEU A 410	74.215 30.453 62.637 1.00 58.30 73.123 29.988 61.713 1.00 61.42	С
ATOM	830 C LEU A 410	73.123 29.988 61.713 1.00 61.42	С
ATOM	831 O LEU A 410	72.240 30.726 61.277 1.00 62.98	Ο
ATOM	832 CB LEU A 410	73.896 30.029 64.080 1.00 60.54	С
ATOM	833 CG LEU A 410	74.877 30.535 65.147 1.00 61.88	С
	834 CD1 LEU A 410	74.560 30.031 66.548 1.00 60.79	С
ATOM	835 CD2 LEU A 410	76.283 30.133 64.745 1.00 62.85	С
ATOM		73.124 28.703 61.379 1.00 64.97	N
ATOM	837 CA ASP A 411	72.121 28.133 60.480 1.00 68.11	С
ATOM	838 C ASP A 411	71.349 27.042 61.208 1.00 70.80	С
ATOM	839 O ASP A 411	71.717 26.692 62.323 1.00 68.64	0
ATOM	840 CB ASP A 411	72 772 27 554 59 224 1.00 66.57	C
ATOM	841 CG ASP A 411	73.750 26.453 59.578 1.00 67.45 73.421 25.590 60.428 1.00 67.96	С
ATOM	842 OD1 ASP A 411	73.421 25.590 60.428 1.00 67.96	0
	843 OD2 ASP A 411	74.874 26.446 59.021 1.00 67.41	0
ATOM	844 N ARG A 412	70.306 26.527 60.583 1.00 78.02	N
ATOM	845 CA ARG A 412	69.449 25.494 61.180 1.00 83.69	С
ATOM	846 C ARG A 412		С
ATOM	847 O ARG A 412	69.998 24.217 63.162 1.00 81.46	0
ATOM	848 CB ARG A 412	68.604 24.859 60.063 1.00 88.30	С
ATOM	849 CG ARG A 412	67.453 23.982 60.525 1.00 95.09	С
ATOM	850 CD ARG A 412	67.522 22.612 59.901 1.00101.21	С
ATOM	851 NE ARG A 412	67.033 21.492 60.685 1.00106.04	N
ATOM	852 CZ ARG A 412	67.081 20.221 60.269 1.00109.24	С
ATOM	853 NH1 ARG A 412	67.593 19.906 59.082 1.00110.96	N
ATOM	854 NH2 ARG A 412	66.610 19.256 61.058 1.00110.83	N
ATOM	855 N ASN A 413	71.187 23.790 61.345 1.00 86.77	N
ATOM	856 CA ASN A 413	71.997 22.750 61.947 1.00 88.40	С
ATOM		72,726 23.186 63.197 1.00 86.70	С
ATOM	858 O ASN A 413	72.770 22.446 64.194 1.00 84.78	0
ATOM	859 CB ASN A 413	73.003 22.181 60.930 1.00 94.30	С
ATOM	860 CG ASN A 413	73.815 21.042 61.513 1.00 98.85	С
ATOM	861 OD1 ASN A 413	73.568 20.563 62.622 1.00102.19	0
ATOM	862 ND2 ASN A 413	74.833 20.518 60.837 1.00101.25	N
ATOM	863 N GLN A 414	73.361 24.370 63.167 1.00 85.09	N
ATOM		73.997 24.886 64.392 1.00 82.79	С
ATOM		72.984 25.035 65.518 1.00 81.33	С
ATOM		73.180 24.679 66.682 1.00 79.48	O
ATOM	867 CB GLN A 414	74.664 26.220 64.092 1.00 81.91	C
ATOM	868 CG GLN A 414	76.063 26.114 63.538 1.00 82.77	C
ATOM		76.431 27.257 62.620 1.00 84.68	C
Y I OIM	509 CD GLIVATIA	7 G. 13 L 27.257 G2.Q20 1.00 G4.00	_

0 75.687 27.652 61.712 1.00 85.74 870 OE1 GLN A 414 **ATOM** 77.608 27.859 62.821 1.00 85.01 N 871 NE2 GLN A 414 **ATOM** 71.781 25.527 65.216 1.00 80.63 N 872 N GLY A 415 ATOM 70.742 25.696 66.201 1.00 83.40 C 873 CA GLY A 415 ATOM C 70.340 24.445 66.944 1.00 83.82 874 C GLY A 415 **ATOM** 0 69.712 24.503 68.003 1.00 84.09 875 O GLY A 415 ATOM N 70.653 23.278 66.432 1.00 86.07 876 N LYS A 416 **ATOM** C 70.358 21.991 67.041 1.00 88.46 877 CA LYS A 416 ATOM C 71.346 21.617 68.133 1.00 90.69 878 C LYS A 416 **ATOM** 0 71.114 20.736 68.976 1.00 90.97 879 O LYS A 416 **ATOM** 70.292 20.922 65.936 1.00 86.72 C 880 CB LYS A 416 ATOM 72.472 22.326 68.256 1.00 92.64 N 885 N CYS A 417 ATOM 73.483 22.108 69.272 1.00 93.07 C 886 CA CYS A 417 ATOM 72.909 22.354 70.666 1.00 93.38 C 887 C CYS A 417 ATOM 0 73.434 21.863 71.658 1.00 92.91 888 O CYS A 417 ATOM 74.701 22.998 69.048 1.00 94.33 C 889 CB CYS A 417 ATOM S 75.678 22.635 67.566 1.00 99.02 890 SG CYS A 417 ATOM N 71.834 23.132 70.752 1.00 93.78 891 N VAL A 418 ATOM C 71.120 23.402 71.968 1.00 93.62 892 CA VAL A 418 ATOM C 69.808 22.596 72.013 1.00 93.64 893 C VAL A 418 ATOM 69.181 22.351 70.999 1.00 91.80 0 894 O VAL A 418 ATOM 70.736 24.892 72.107 1.00 93.31 C 895 CB VAL A 418 ATOM 70.086 25.187 73.456 1.00 91.67 C 896 CG1 VAL A 418 ATOM 71.979 25.742 71.931 1.00 94.17 C 897 CG2 VAL A 418 ATOM 69.412 22.265 73.215 1.00 95.05 N 898 N GLU A 419 ATOM 68.188 21.657 73.643 1.00 95.54 C 899 CA GLU A 419 **ATOM** 66.973 22.239 72.923 1.00 95.38 C 900 C GLU A 419 ATOM 66.476 23.327 73.242 1.00 95.98 0 901 O GLU A 419 ATOM 67.991 21.962 75.166 1.00 95.46 C 902 CB GLU A 419 **ATOM** 66.498 21.521 71.918 1.00 94.14 N 907 N GLY A 420 ATOM C 65.357 21.884 71.143 1.00 92.12 908 CA GLY A 420 **ATOM** C 65.092 23.320 70.781 1.00 89.03 909 C GLY A 420 **ATOM** 64.020 23.850 71.107 1.00 88.17 0 910 O GLY A 420 **ATOM** N 66.033 23.982 70.089 1.00 86.43 911 N MET A 421 **ATOM** C 65.784 25.373 69.683 1.00 82.99 912 CA MET A 421 **ATOM** C 65,464 25,306 68,175 1,00 80,42 913 C MET A 421 **ATOM** 64,989 26,266 67.583 1.00 80.10 o 914 O MET A 421 **ATOM** 66.764 26.427 70.019 1.00 81.48 C 915 CB MET A 421 ATOM C 68,244 26,357 69,911 1.00 79.85 916 CG MET A 421 **ATOM** 69.040 27.989 69.709 1.00 77.79 S 917 SD MET A 421 ATOM C 68.655 28.724 71.288 1.00 79.07 918 CE MET A 421 **ATOM** 65.609 24.092 67.625 1.00 76.08 N 919 N VAL A 422 **ATOM** C 65.334 23.826 66.229 1.00 71.68 920 CA VAL A 422 **ATOM** 63.966 24.412 65.856 1.00 67.41 C 921 C VAL A 422 ATOM 0 63.776 25.123 64.899 1.00 67.37 922 O VAL A 422 ATOM C 65.173 22.322 65.867 1.00 72.40 923 CB VAL A 422 ATOM C 65.967 22.025 64.609 1.00 71.96 924 CG1 VAL A 422 ATOM C 65.512 21.394 67.006 1.00 73.60 925 CG2 VAL A 422 ATOM N 63.017 24.009 66.669 1.00 64.30 926 N GLU A 423 ATOM

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ATOM	927 CA GLU A 423		С
ATOM	928 C GLU A 423	61.457 25.875 66.421 1.00 56.63	С
ATOM	929 O GLU A 423		0
ATOM	930 CB GLU A 423		С
ATOM	931 CG GLU A 423	61.513 22.419 68.085 1.00 76.48	С
ATOM	932 CD GLU A 423	61.053 21.478 66.981 1.00 83.18	С
ATOM	933 OE1 GLU A 423	61.030 21.792 65.757 1.00 84.19	0
ATOM	934 OE2 GLU A 423	60.693 20.332 67.375 1.00 87.12	0
ATOM	935 N ILE A 424	62.064 26.591 67.362 1.00 50.66	N
ATOM	936 CA ILE A 424	62.014 28.050 67.353 1.00 49.94	С
ATOM	937 C ILE A 424	62.833 28.671 66.258 1.00 49.72	С
ATOM	938 O ILE A 424	62.454 29.564 65.483 1.00 47.07	Ο
ATOM	939 CB ILE A 424	62,365 28.585 68.734 1.00 49.44	С
ATOM	940 CG1 ILE A 424	61.957 27.488 69.748 1.00 47.25	С
ATOM	941 CG2 ILE A 424	61.546 29.853 68.939 1.00 52.10	С
ATOM	942 CD1 ILE A 424	61.539 28.004 71.086 1.00 46.42	С
ATOM	943 N PHE A 425	64.032 28.110 66.119 1.00 48.71	N
ATOM	944 CA PHE A 425	64.956 28.558 65.078 1.00 48.83	С
ATOM	945 C PHE A 425	64.259 28.554 63.730 1.00 49.83	С
ATOM	946 O PHE A 425	64,333 29.486 62.912 1.00 49.75	Ο
ATOM	947 CB PHE A 425	66.079 27.557 65.115 1.00 52.26	С
AŤOM	948 CG PHE A 425	67.384 28.056 64.616 1.00 54.82	С
ATOM	949 CD1 PHE A 425	67.534 28.250 63.249 1.00 55.00	C
ATOM	950 CD2 PHE A 425	68,429 28.309 65.493 1.00 54.48	С
ATOM	951 CEI PHE A 425	68.734 28.713 62.751 1.00 54.74	С
ATOM	952 CE2 PHE A 425	69.630 28.763 64.995 1.00 54.33	С
ATOM	953 CZ PHE A 425	69.769 28.957 63.628 1.00 55.26	С
ATOM	954 N ASP A 426	63.592 27.439 63.451 1.00 50.34	N
ATOM	955 CA ASP A 426	62.830 27.302 62.211 1.00 52.02	С
ATOM	956 C ASP A 426	61.741 28.379 62.154 1.00 47.88	С
ATOM	957 O ASP A 426	61.620 29.141 61.192 1.00 45.05	Ο
ATOM	958 CB ASP A 426	62.232 25.927 62.120 1.00 58.40	С
ATOM	959 CG ASP A 426	63.114 24.758 61.823 1.00 62.55	С
ATOM	960 OD1 ASP A 426		0
ATOM	961 OD2 ASP A 426		0
ATOM	962 N MET A 427		N
ATOM	963 CA MET A 427		С
ATOM	964 C MET A 427		С
ATOM	965 O MET A 427		0
ATOM	966 CB MET A 427		С
ATOM	967 CG MET A 427		С
ATOM	968 SD MET A 427	57.470 28.508 66.400 1.00 51.78	S
ATOM	969 CE MET A 427	58.854 28.059 67.403 1.00 45.57	С
ATOM	970 N LEUA 428	61.653 31.212 63.699 1.00 37.72	N
ATOM	971 CA LEU A 428		С
ATOM	972 C LEU A 428	62.778 32.561 62.036 1.00 36.86	С
ATOM	973 O LEU A 428		Ο
ATOM	974 CB LEU A 428		С
ATOM	975 CG LEU A 428		С
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ATOM	976 CD1 LEU A 428	64.057 32.285 66.969 1.00 36.73	C
ATOM	977 CD2 LEU A 428	62.723 34.177 66.125 1.00 37.83	С
ATOM		63.240 31.432 61.475 1.00 40.60	N
ATOM	979 CA LEU A 429	63.706 31.476 60.065 1.00 41.29	С
ATOM		62.605 31.928 59.145 1.00 39.00	C
ATOM		62.720 32.870 58.371 1.00 39.51	0
ATOM		64.313 30.144 59.690 1.00 43.27	С
ATOM	983 CG LEU A 429	65.812 30.002 59.966 1.00 45.30	C
ATOM	984 CD1 LEU A 429	66.293 28.587 59.649 1.00 45.70	С
ATOM	985 CD2 LEU A 429	66.629 31.027 59.197 1.00 43.74	С
ATOM	986 N ALA A 430	61.448 31.309 59.364 1.00 39.75	N
ATOM	987 CA ALA A 430	60.243 31.583 58.587 1.00 37.09	C
ATOM	988 C ALA A 430	59.798 33.011 58.767 1.00 38.56	С
ATOM	989 O ALA A 430	59.521 33.697 57.752 1.00 38.33	0
ATOM	990 CB ALA A 430	59.208 30.593 59.021 1.00 39.99	C
ATOM		59.882 33.500 60.028 1.00 35.59	N
ATOM		59,549 34,937 60.144 1.00 36.46	С
ATOM	993 C THR A 431	60,428 35.826 59.333 1.00 37.93	С
ATOM	994 O THR A 431	59.934 36.643 58.554 1.00 38.61	0
ATOM		59.488 35.351 61.600 1.00 36.66	С
ATOM	996 OG1 THR A 431	58,696 34,368 62,308 1.00 44.00	0
ATOM	997 CG2 THR A 431	58,908 36.711 61.812 1.00 32.95	С
ATOM		61.781 35.804 59.328 1.00 43.67	N
ATOM		62.459 36.829 58.499 1.00 45.86	С
ATOM	1000 C SER A 432	62.140 36.599 57.029 1.00 45.06	С
ATOM	1001 O SER A 432	62.151 37.499 56.200 1.00 40.01	0
ATOM	1002 CB SER A 432	63.961 37.037 58.613 1.00 45.04	С
ATOM		64.652 35.870 58.844 1.00 44.31	Ο
ATOM	1004 N SER A 433	61.942 35.297 56.773 1.00 47.09	N
ATOM	1005 CA SER A 433	61.611 35.007 55.384 1.00 49.54	С
ATOM	1006 C SER A 433	60.360 35.760 54.981 1.00 49.50	С
ATOM		60.276 36.385 53.896 1.00 51.37	Ο
ATOM		61.533 33.492 55.255 1.00 50.61	С
ATOM	1009 OG SER A 433	61.782 33.268 53.861 1.00 58.03	0
	1010 N ARG A 434	59,359 35.767 55.868 1.00 45.71	N
		58.112 36.442 55.471 1.00 45.67	С
		58.365 37.904 55.424 1.00 45.99	С
	1013 O ARG A 434	57.741 38.684 54.686 1.00 48.03	Ο
	1014 CB ARG A 434	56,994 35.888 56.328 1.00 52.87	С
	1015 CG ARG A 434	55.825 36.768 56.669 1.00 61.64	С
	1016 CD ARG A 434	54.448 36.253 56.247 1.00 65.66	С
	1017 NE ARG A 434		N
	1018 CZ ARG A 434	52,755 37,777 55,178 1.00 74,32	С
	1019 NH1 ARG A 434	51.884 37.683 56.194 1.00 76.56	N
	1020 NH2 ARG A 434	52.466 38.531 54.113 1.00 72.73	N
	1021 N PHE A 435	59.278 38.400 56.271 1.00 45.66	N
	1022 CA PHE A 435	59.591 39.822 56.251 1.00 46.91	C
ATOM		60.212 40.184 54.893 1.00 44.85	C
ATOM		60.006 41.239 54.325 1.00 45.13	Ō
ATOM	1024 O 11112 11 433	00,000 TI,207 J 1,023 T.00 10120	_

60.586 40.207 57.352 1.00 48.27 C ATOM 1025 CB PHE A 435 59.982 40.529 58.672 1.00 51.19 C ATOM 1026 CG PHE A 435 58.604 40.442 58.870 1.00 53.63 C ATOM 1027 CD1 PHE A 435 C ATOM 1028 CD2 PHE A 435 60.782 40.922 59.746 1.00 47.96 ATOM 1029 CE1 PHE A 435 58.025 40.713 60.097 1.00 52.73 C ATOM 1030 CE2 PHE A 435 60.194 41.181 60.955 1.00 47.26 58.840 41.076 61.157 1.00 48.94 ATOM 1031 CZ PHE A 435 N ATOM 1032 N ARG A 436 61.056 39.323 54.400 1.00 47.63 ATOM 1033 CA ARG A 436 61.746 39.482 53.124 1.00 49.34 C ATOM 1034 C ARG A 436 60.645 39.474 52.078 1.00 49.53 C ATOM 1035 O ARG A 436 60.330 40.477 51.451 1.00 45.06 0 62.682 38.315 52.896 1.00 50.60 C ATOM 1036 CB ARG A 436 ATOM 1037 CG ARG A 436 63.939 38.648 52.124 1.00 56.76 ATOM 1038 CD ARG A 436 64.616 37.327 51.713 1.00 61.86 ATOM 1039 NE ARG A 436 65.061 36.607 52.886 1.00 66.94 N ATOM 1040 CZ ARG A 436 64.776 35.363 53.238 1.00 70.98 C ATOM 1041 NH1 ARG A 436 63.978 34.637 52.445 1.00 72.78 ATOM 1042 NH2 ARG A 436 65.262 34.887 54.395 1.00 71.17 N ATOM 1043 N MET A 437 59.931 38.317 52.119 1.00 53.08 N ATOM 1044 CA MET A 437 58.819 38.277 51.152 1.00 57.01 C ATOM 1045 C MET A 437 58.080 39.607 51.214 1.00 55.26 C ATOM 1046 O MET A 437 58.069 40.283 50.197 1.00 57.39 0 ATOM 1047 CB MET A 437 57.941 37.108 51.344 1.00 63.52 C ATOM 1048 CG MET A 437 58.313 35.727 50.890 1.00 71.66 C ATOM 1049 SD MET A 437 57.582 34.534 52.062 1.00 84.11 ATOM 1050 CE MET A 437 55.865 35.144 52.090 1.00 79.21 C ATOM 1051 N MET A 438 57,523 40.091 52,326 1.00 51.51 N 56.773 41.324 52.297 1.00 51.37 C ATOM 1052 CA MET A 438 ATOM 1053 C MET A 438 57.538 42.607 52.026 1.00 50.12 C 56.893 43.685 51.973 1.00 48.99 0 ATOM 1054 O MET A 438 ATOM 1055 CB MET A 438 56.028 41.518 53.621 1.00 52.61 ATOM 1056 CG MET A 438 55.222 40.334 54.061 1.00 54.98 54.439 40.648 55.643 1.00 59.57 S ATOM 1057 SD MET A 438 C ATOM 1058 CE MET A 438 53.926 42.358 55.466 1.00 55.04 ATOM 1059 N ASN A 439 58.846 42.523 51.964 1.00 48.54 N ATOM 1060 CA ASN A 439 59.767 43.614 51.794 1.00 45.77 C 59.605 44.567 52,968 1.00 42.78 C ATOM 1061 C ASN A 439 59.522 45.787 52.761 1.00 39.35 0 ATOM 1062 O ASN A 439 ATOM 1063 CB ASN A 439 59.622 44.374 50.518 1.00 53.65 C 60.859 45.147 50.093 1.00 60.47 ATOM 1064 CG ASN A 439 61.779 45.547 50.798 1.00 58.68 0 ATOM 1065 OD1 ASN A 439 ATOM 1066 ND2 ASN A 439 60.875 45.410 48.768 1.00 65.24 N ATOM 1067 N LEU A 440 59.545 43.937 54.172 1.00 39.68 N ATOM 1068 CA LEU A 440 59.363 44.798 55.341 1.00 40.85 C ATOM 1069 C LEU A 440 60.302 45.992 55.289 1.00 40.66 C ATOM 1070 O LEU A 440 61.439 45.917 54.837 1.00 40.49 0 ATOM 1071 CB LEU A 440 59.506 44.052 56.677 1.00 42.20 C ATOM 1072 CG LEU A 440 59.201 45.057 57.839 1.00 43.75 C ATOM 1073 CD1 LEU A 440 57.802 45.601 57.642 1.00 45.00

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ATOM	1074	CD2 LEU A 440	59.380 44.431 59.202 1.00 42.76	С
ATOM	1075	N GLN A 441	59.881 47.156 55.736 1.00 42.17	N
ATOM	1076	CA GLN A 441	60.755 48.326 55.684 1.00 42.54	C
ATOM	1077	C GLN A 441	61.111 48.837 57.064 1.00 45.77	С
ATOM	1078	O GLN A 441	60.289 48.917 57.992 1.00 46.95	0
ATOM	1079	CB GLN A 441	59.947 49.392 54.913 1.00 44.80	С
ATOM	1080	CG GLN A 441	59.648 48.869 53.469 1.00 46.60	C
ATOM	1081	CD GLN A 441	60.870 49.261 52.620 1.00 46.29	C
ATOM	1082	OE1 GLN A 441	61.209 50.473 52.644 1.00 43.94	0
ATOM		NE2 GLN A 441	61.391 48.217 51.988 1.00 43.50	N
ATOM	1084	N GLY A 442	62.361 49.221 57.240 1.00 44.76	N
ATOM	1085	CA GLY A 442	62.942 49.758 58.436 1.00 41.75	C
ATOM	1086	C GLY A 442	61.971 50.542 59.255 1.00 41.41	С
ATOM	1087	O GLY A 442	61.661 50.119 60.370 1.00 43.47	0
ATOM	1088	N GLU A 443	61.418 51.600 58.688 1.00 43.44	N
ATOM	1089	CA GLU A 443	60.442 52.464 59.287 1.00 43.18	С
ATOM	1090	C GLU A 443	59.181 51.714 59.768 1.00 41.51	С
ATOM	1091	O GLU A 443	58.536 52.266 60.688 1.00 41.33	0
ATOM	1092	CB GLU A 443	60.005 53.585 58.352 1.00 45.30	С
ATOM	1093	CG GLU A 443	60.996 54.545 57.786 1.00 46.12	C
	1094	CD GLU A 443	61.854 53.906 56.720 1.00 51.40	С
ATOM		OE1 GLU A 443	61,523 52.818 56.225 1.00 51.51	0
ATOM	1096	OE2 GLU A 443	62.932 54.443 56.343 1.00 57.58	0
ATOM			58.830 50.580 59.194 1.00 37.35	N
ATOM		CA GLU A 444	57.661 49.801 59.612 1.00 38.11	С
ATOM	1099	C GLU A 444	58.071 48.899 60.782 1.00 36.47	С
ATOM	1100	O GLU A 444	57.364 48.667 61.760 1.00 40.60	Ο
ATOM	1101	CB GLU A 444	57.126 48.855 58.543 1.00 40.40	С
ATOM	1102	CG GLU A 444	56.654 49.456 57.251 1.00 43.75	C
ATOM	1103	CD GLU A 444	56.171 48.486 56.187 1.00 44.27	С
ATOM	1104	OE1 GLU A 444	56.948 47.714 55.593 1.00 42.90	0
ATOM	1105	OE2 GLU A 444	54.945 48.547 55.928 1.00 43.73	0
ATOM	1106	N PHE A 445	59.274 48.392 60.688 1.00 36.90	N
ATOM	1107	CA PHE A 445	59.910 47.530 61.676 1.00 36.32	C
ATOM	1108	C PHE A 445	59.990 48.218 63.020 1.00 38.08	С
ATOM	1109	O PHE A 445	59.624 47.708 64.078 1.00 43.18	0
ATOM	1110	CB PHE A 445	61.324 47.215 61.222 1.00 33.88	С
ATOM	1111	CG PHE A 445	62.219 46.649 62.240 1.00 34.44	С
ATOM	1112	CD1 PHE A 445	62.075 45.370 62.709 1.00 33.30	С
ATOM	1113	CD2 PHE A 445	63.265 47.438 62.742 1.00 35.81	С
ATOM	1114	CE1 PHE A 445	62.975 44.855 63.646 1.00 35.64	С
ATOM	1115	CE2 PHE A 445	64.199 46.911 63.618 1.00 34.03	С
ATOM	1116	CZ PHE A 445	64.031 45.624 64.090 1.00 33.63	С
		N VAL A 446	60.370 49.468 62.998 1.00 36.38	N
		CA VAL A 446	60.501 50.229 64.260 1.00 35.39	С
		C VAL A 446	59.160 50.513 64.836 1.00 36.39	С
		O VAL A 446	58.899 50.721 66.060 1.00 36.88	Ο
ATOM			61.340 51.422 63.743 1.00 37.96	С
		CG1 VAL A 446	61.016 52.732 64.350 1.00 36.13	С

62.806 51.032 63.810 1.00 36.84 C ATOM 1123 CG2 VAL A 446 N 58.166 50.587 63.959 1.00 38.09 ATOM 1124 N CYS A 447 56.756 50.836 64.384 1.00 36.81 C ATOM 1125 CA CYS A 447 56.242 49.584 65.066 1.00 35.90 C ATOM 1126 C CYS A 447 55.686 49.628 66.147 1.00 36.40 0 ATOM 1127 O CYS A 447 56.001 51.134 63.134 1.00 39.05 C ATOM 1128 CB CYS A 447 S 55.897 52.861 62.706 1.00 45.24 ATOM 1129 SG CYS A 447 56.515 48.431 64.448 1.00 37.34 N ATOM 1130 N LEU A 448 56.179 47.116 65.016 1.00 36.19 ATOM 1131 CA LEU A 448 C C ATOM 1132 C LEU A 448 56.884 46.877 66.333 1.00 35.93 56.332 46.318 67.303 1.00 36.91 O ATOM 1133 O LEU A 448 C 56.644 46.016 64.059 1.00 37.42 ATOM 1134 CB LEU A 448 C 55.919 45.875 62.723 1.00 38.60 ATOM 1135 CG LEU A 448 56.204 44.485 62.166 1.00 38.61 C ATOM 1136 CD1 LEU A 448 C ATOM 1137 CD2 LEU A 448 54.407 46.000 62.875 1.00 38.37 58.161 47.327 66.475 1.00 34.08 N ATOM 1138 N LYS A 449 C ATOM 1139 CA LYS A 449 58.759 47.056 67.800 1.00 33.35 58.051 47.861 68.885 1.00 32.12 C ATOM 1140 C LYS A 449 0 57.772 47.421 69.977 1.00 31.98 ATOM 1141 O LYS A 449 C 60.222 47.413 67.867 1.00 35.64 ATOM 1142 CB LYS A 449 C 61.196 46.311 67.540 1.00 40.11 ATOM 1143 CG LYS A 449 C 62,593 46,562 68.113 1.00 37.82 ATOM 1144 CD LYS A 449 63.209 47.746 67.359 1.00 39.59 C ATOM 1145 CE LYS A 449 64,552 48,079 67,932 1.00 45.13 N ATOM 1146 NZ LYS A 449 57.796 49.148 68.608 1.00 32.09 N ATOM 1147 N SER A 450 C 57.214 49.985 69.643 1.00 32.69 ATOM 1148 CA SER A 450 C ATOM 1149 C SER A 450 55.872 49.379 70.046 1.00 35.21 55.572 49.405 71.237 1.00 35.15 O ATOM 1150 O SER A 450 C ATOM 1151 CB SER A 450 57.093 51.427 69.253 1.00 33.33 0 58.301 51.920 68.712 1.00 44.51 ATOM 1152 OG SER A 450 55.152 48.892 69.015 1.00 31.47 N ATOM 1153 N ILE A 451 53.871 48.281 69.300 1.00 29.67 C ATOM 1154 CA ILE A 451 54.073 47.088 70.212 1.00 29.71 C ATOM 1155 C ILE A 451 0 53.319 46.948 71.179 1.00 30.52 ATOM 1156 O ILE A 451 C ATOM 1157 CB ILE A 451 53.185 47.857 67.987 1.00 30.16 ATOM 1158 CG1 ILE A 451 52.654 49.104 67.276 1.00 29.31 C C 52.097 46.805 68.217 1.00 25.93 ATOM 1159 CG2 ILE A 451 C 52.274 48.796 65.821 1.00 32.04 ATOM 1160 CD1 ILE A 451 N 55.075 46.229 69.918 1.00 28.54 ATOM 1161 N ILE A 452 55.300 45.060 70.761 1.00 25.63 C ATOM 1162 CA ILE A 452 C 55.576 45.545 72.180 1.00 30.38 ATOM 1163 C ILE A 452 0 55.079 45.005 73.137 1.00 34.58 ATOM 1164 O ILE A 452 56.469 44.234 70.281 1.00 26.82 ATOM 1165 CB ILE A 452 С 56.170 43.518 68.957 1.00 30.90 C ATOM 1166 CG1 ILE A 452 57.009 43.259 71.314 1.00 21.12 C ATOM 1167 CG2 ILE A 452 C 57.349 42.688 68.405 1.00 25.51 ATOM 1168 CD1 ILE A 452 N 56.367 46.581 72.361 1.00 32.06 ATOM 1169 N LEU A 453 C 56.675 47.098 73.654 1.00 34.04 ATOM 1170 CA LEU A 453 C 55,436 47,537 74,371 1.00 34,53 ATOM 1171 C LEU A 453

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ATOM	1172 O LEU A 453	55.177 47.100 75.495 1.00 40.58	Ο
ATOM	1173 CB LEU A 453	57.676 48.265 73.594 1.00 33.55	С
ATOM	1174 CG LEU A 453	57.973 48.870 74.984 1.00 31.37	С
ATOM	1175 CD1 LEU A 453	58.292 47.746 75.949 1.00 27.35	С
ATOM	1176 CD2 LEU A 453	58.980 49.992 74.961 1.00 26.50	С
ATOM	1177 N LEU A 454	54.627 48.386 73.806 1.00 35.04	N
ATOM		53.404 48.815 74.482 1.00 35.08	С
ATOM	1179 C LEU A 454	52.313 47.814 74.641 1.00 37.41	С
ATOM	1180 O LEU A 454	51.468 47.943 75.510 1.00 36.19	0
ATOM		52.775 49.973 73.645 1.00 32.94	С
ATOM		53.728 51.185 73.576 1.00 34.24	С
	1183 CD1 LEU A 454	53.055 52.297 72.825 1.00 32.61	С
ATOM	1184 CD2 LEU A 454	54.126 51.597 74.987 1.00 34.42	С
ATOM	1185 N ASN A 455	52.180 46.850 73.728 1.00 42.96	N
ATOM		51.060 45.936 73.771 1.00 44.63	С
ATOM	1187 C ASN A 455		С
ATOM	1188 O ASN A 455	50.303 44.023 74.961 1.00 52.94	0
ATOM	1189 CB ASN A 455		С
ATOM	1190 CG ASN A 455	49.596 44.620 72.164 1.00 43.46	С
ATOM	1191 OD1 ASN A 455	49.696 43.551 71.583 1.00 42.54	Ο
ATOM	1192 ND2 ASN A 455	48.475 45.034 72.727 1.00 46.97	N
ATOM	1193 N SER A 456	52.395 44.046 74.548 1.00 50.76	N
ATOM		52.427 42.713 75.145 1.00 53.37	С
ATOM	1195 C SER A 456	52.032 42.695 76.583 1.00 56.18	С
ATOM	1196 O SER A 456	51.549 41.691 77.113 1.00 56.74	0 .
ATOM	1197 CB SER A 456	53.794 42.093 74.786 1.00 52.37	С
ATOM	1198 OG SER A 456		0
ATOM	1199 N GLY A 457	52.241 43.761 77.316 1.00 61.86	N
ATOM	1200 CA GLY A 457	51,997 43.862 78.731 1.00 70.54	С
ATOM	1201 C GLY A 457		С
ATOM	1202 O GLY A 457		Ο
ATOM	1203 N VAL A 458		N
ATOM	1204 CA VAL A 458	48.987 46.195 78.378 1.00 90.25	С
ATOM	1205 C VAL A 458	47.897 45.551 79.210 1.00 96.24	C
	1206 O VAL A 458	46,948 46,250 79,609 1,00 98,11	0
	1207 CB VAL A 458	48.448 46.636 76.990 1.00 89.27	С
	1208 CG1 VAL A 458	47.739 45.491 76.289 1.00 89.46	С
	1209 CG2 VAL A 458	47.547 47.845 77.079 1.00 88.97	С
	1210 N TYR A 459	47,924 44.257 79.513 1.00101.74	N
	1211 CA TYR A 459	46.973 43.497 80.269 1.00104.80	С
	1212 C TYR A 459	47.332 43.286 81.740 1.00105.22	С
	1213 O TYR A 459	47.016 42.180 82.231 1.00105.07	0
	1214 CB TYR A 459	46.814 42.080 79.662 1.00107.02	С
	1215 CG TYR A 459	45.822 42.038 78.519 1.00110.17	С
	1216 CD1 TYR A 459	45.419 43.212 77.893 1.00110.98	С
	1217 CD2 TYR A 459	45.308 40.830 78.053 1.00110.39	C
	1217 CB2 TTR A 459	44.545 43.205 76.835 1.00112.30	Č
	1219 CE2 TYR A 459		C
	1219 CZZ TYR A 459	44.051 42.000 76.399 1.00112.88	C
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ATOM 1221 OH TYR A 459	43.168 41.991 75.347 1.00115.80	Ο
ATOM 1222 N GLU A 470	43.165 56.078 83.507 1.00107.33	N
ATOM 1223 CA GLU A 470	43.526 57.004 82.435 1.00107.02	С
ATOM 1224 C GLU A 470	44.890 56.630 81.849 1.00105.48	С
ATOM 1225 O GLU A 470	45.363 57.299 80.943 1.00106.09	Ο
ATOM 1226 CB GLU A 470	43.575 58.456 82.919 1.00106.27	С
ATOM 1231 N GLU A 471	45.492 55.590 82.396 1.00103.12	N
ATOM 1232 CA GLU A 471	46.801 55.140 81.925 1.00101.16	С
ATOM 1232 C/1 G26 17 17 1	46.592 54.169 80.779 1.00 99.18	С
ATOM 1234 O GLU A 471	47.055 54.348 79.647 1.00 99.80	0
ATOM 1234 C GLU A 471	47.605 54.547 83.076 1.00101.62	С
ATOM 1240 N LYS A 472	45.728 53.170 81.002 1.00 95.72	N
ATOM 1240 K 21511 112 ATOM 1241 CA LYS A 472	45.352 52.182 79.990 1.00 88.76	С
	45.036 52.984 78.727 1.00 84.43	С
ATOM 1242 C LYS A 472 ATOM 1243 O LYS A 472	45.594 52.757 77.666 1.00 85.42	O
ATOM 1243 O LTS A 472	44.096 51.416 80.408 1.00 89.61	С
	44.145 53.954 78.913 0.50 80.32	N
	44.142 53.947 78.917 0.50 81.68	N
ATOM 1250 N BASP A 473 ATOM 1251 CA AASP A 473	43.735 54.858 77.861 0.50 76.63	С
	43.727 54.830 77.848 0.50 78.99	С
	44.905 55.533 77.166 0.50 72.53	С
	44.863 55.585 77.186 0.50 74.62	С
	44.906 55.645 75.937 0.50 70.54	0
	45.017 55.398 75.961 0.50 73.32	0
	42.788 55.917 78.446 0.50 77.43	С
	42.628 55.750 78.383 0.50 81.54	Č
		С
		C
		C
		C
		C
ATOM 1263 OD2AASP A 473 ATOM 1264 OD2BASP A 473	_	C
ATOM 1265 N. HIS A 474	45.903 55.985 77.921 1.00 70.51	N
	47.039 56.684 77.314 1.00 64.59	С
ATOM 1266 CA HIS A 474	47.754 55.773 76.335 1.00 60.83	C
ATOM 1267 C HIS A 474	47.950 56.109 75.155 1.00 58.49	ŏ
ATOM 1268 O HIS A 474	48.007 57.255 78.327 1.00 64.63	C
ATOM 1269 CB HIS A 474	49.247 57.893 77.753 1.00 66.15	Č
ATOM 1270 CG HIS A 474	49.230 58.987 76.893 1.00 64.28	N
ATOM 1271 ND1 HIS A 474	50.560 57.566 77.949 1.00 63.36	C
ATOM 1272 CD2 HIS A 474	50.461 59.305 76.567 1.00 63.50	Č
ATOM 1273 CE1 HIS A 474	51.263 58.458 77.202 1.00 64.89	N
ATOM 1274 NE2 HIS A 474	48.085 54.566 76.816 1.00 56.86	N
ATOM 1275 N ILE A 475	48.793 53.658 75.933 1.00 56.72	Ċ
ATOM 1276 CA ILE A 475		c
ATOM 1277 C ILE A 475	48.013 53.327 74.667 1.00 57.11	Ö
ATOM 1278 O ILE A 475	48.606 53.228 73.567 1.00 54.05	C
ATOM 1279 CB ILE A 475	49.240 52.385 76.618 1.00 58.11	C
	49.983 52.704 77.908 1.00 60.17	C
ATOM 1281 CG2 ILE A 475	50.144 51.632 75.633 1.00 60.22	C

ATO) (1282 CD1 ILE A 475	50.468 51.438 78.616 1.00 63.03	С
ATOM	1282 CDT ILLE A 475	46.701 53.150 74.800 1.00 55.97	N
ATOM	1284 CA HIS A 476	45.863 52.867 73.648 1.00 58.59	С
ATOM	1285 C HIS A 476	45.863 53.976 72.617 1.00 59.35	С
ATOM		45.714 53.730 71.394 1.00 61.12	0
ATOM	1287 CB HIS A 476	44.463 52.526 74.106 1.00 64.75	С
ATOM	1287 CB 1H3 A 476	44.333 51.131 74.657 1.00 72.37	C
ATOM	1280 ND1 LTS A 476	45.206 50.100 74.365 1.00 73.22	N
ATOM	1290 CD2 HIS A 476		C
ATOM	1291 CE1 HIS A 476		Č
ATOM	1292 NE2 HIS A 476	43.721 49.266 75.694 1.00 74.59	N
ATOM	1293 N ARG A 477	46.135 55.219 73.001 1.00 58.21	N
ATOM	1294 CA ARG A 477	46.136 56.304 72.015 1.00 57.66	C
ATOM	1295 C ARG A 477	47.505 56.399 71.380 1.00 55.49	C
ATOM	1296 O ARG A 477		Ö
ATOM		45.741 57.625 72.644 1.00 62.00	Ċ
ATOM	1297 CB ARG A 477	44.852 57.527 73.864 1.00 66.35	Č
ATOM	1298 CG ARG A 477		č
ATOM	1299 CD ARG A 477	44.206 59.875 73.400 1.00 72.49	N
ATOM	1300 NE ARG A 477	44.206 55.917 72.109 1.00 51.61	N
ATOM	1304 N VAL A 478	49.864 55.952 71.511 1.00 48.31	Ċ
ATOM	1305 CA VAL A 478	49.873 54.851 70.465 1.00 45.77	c
ATOM	1306 C VAL A 478		o ·
ATOM	1307 O VAL A 478		Č
ATOM	1308 CB VAL A 478	52.313 55.702 71.995 1.00 47.97	Č
ATOM	1309 CG1 VAL A 478		č
ATOM	1310 CG2 VAL A 478	49.226 53.747 70.861 1.00 44.03	N
ATOM	1311 N LEU A 479		Ĉ
ATOM	1312 CA LEU A 479	48.311 52.989 68.741 1.00 41.59	c
	1313 C LEU A 479	48.781 52.725 67.618 1.00 45.09	Ö
ATOM	1314 O LEU A 479		. C.
	1315 CB LEU A 479		C
	1316 CG LEU A 479		Č
ATOM			Č
	1318 CD2 LEU A 479	47.211 53.712 68.960 1.00 42.05	N
	1319 N ASP A 480 1320 CA ASP A 480		C
	1321 C ASP A 480	47.374 55.147 66.986 1.00 42.83	c
		47.305 55.139 65.748 1.00 42.30	Ö
	1322 O ASP A 480	45.201 54.953 68.099 1.00 42.23	C
	1323 CB ASP A 480	the state of the s	Č
	1324 CG ASP A 480	_	o
	1325 OD1 ASP A 480		Ö
ATOM	1326 OD2 ASP A 480	48.194 55.938 67.729 1.00 41.96	N
	1327 N LYS A 481	49.063 56.824 66.929 1.00 44.36	Ċ
	1328 CA LYS A 481	50.015 55.990 66.111 1.00 39.42	c
	1329 C LYS A 481	50.178 56.356 64.967 1.00 40.40	Ö
	1330 O LYS A 481	49.767 57.875 67.765 1.00 50.78	C
ATOM			Č
ATOM	1332 CG LYS A 481		Č
ATOM	1333 CD LYS A 481	50.362 60.262 67.571 1.00 59.84	C

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ATOM	1334	CE LYS A 481	50.299 61.305 66.443 1.00 64.03	С
ATOM	1335	NZ LYS A 481	48.891 61.472 65.919 1.00 65.06	N
ATOM	1336	N ILE A 482	50.585 54.906 66.617 1.00 37.30	N
ATOM	1337	CA ILE A 482	51.484 54.115 65.740 1.00 37.67	С
ATOM	1338	C ILE A 482	50.784 53.474 64.576 1.00 37.39	С
ATOM	1339	O ILE A 482	51.369 53.361 63.504 1.00 40.01	0
ATOM	1340	CB ILE A 482	52.223 53.033 66.573 1.00 38.51	С
	1341	CG1 ILE A 482	52.717 53.713 67.841 1.00 37.12	С
		CG2 ILE A 482	53.229 52.354 65.681 1.00 32.84	С
ATOM		CD1 ILE A 482	53.464 52.910 68.842 1.00 36.63	C
ATOM	1344	N THR A 483	49.541 53.024 64.688 1.00 37.56	N
ATOM	1345	CA THR A 483	48.801 52.521 63.553 1.00 38.49	С
ATOM	1346	C THR A 483	48.707 53.631 62.498 1.00 41.74	С
ATOM	1347	O THR A 483	49.115 53.398 61.323 1.00 41.89	0
ATOM	1348	CB THR A 483	47.358 52.105 63.878 1.00 39.30	С
ATOM	1349	OG1 THR A 483	47.465 50.929 64.705 1.00 40.84	0
	1350	CG2 THR A 483	46.655 51.747 62.564 1.00 36.88	С
			48.231 54.813 62.941 1.00 43.21	N
ATOM		CA ASP A 484	48.226 55.987 62.034 1.00 43.09	С
ATOM	1353		49.567 56.088 61.303 1.00 42.19	С
	1354		49,591 56.087 60.048 1.00 43.92	0
		CB ASP A 484	48.063 57.317 62.737 1.00 43.77	С
		CG ASP A 484	46.749 57.475 63.456 1.00 47.64	С
				0
		OD2 ASP A 484		0
		N THR A 485	50.645 56.123 62.071 1.00 39.45	N
ATOM		CA THR A 485	51.990 56.225 61.436 1.00 40.57	С
ATOM	1361	C THR A 485	52.253 55.079 60.500 1.00 40.59	С
ATOM	1362	O THR A 485	52.717 55.274 59.365 1.00 44.93	0
ATOM			53.104 56.279 62.489 1.00 39.40	С
ATOM	1364	OG1 THR A 485	52.575 56.995 63.625 1.00 35.82	0
ATOM	1365		54.377 56.779 61.950 1.00 34.78	С
ATOM		N LEU A 486		N
		CA LEU A 486	52.127 52.729 59.939 1.00 43.09	С
		C LEU A 486	51.312 52.966 58.681 1.00 40.80	С
		O LEU A 486	51.781 52.838 57.558 1.00 38.70	0
			51.755 51.499 60.688 1.00 42.99	С
			52.613 50.294 60.838 1.00 44.81	С
		CD1 LEU A 486		С
		CD2 LEU A 486		С
		N ILE A 487	50.040 53.365 58.786 1.00 42.87	N
		CA ILE A 487	49.240 53.582 57.545 1.00 44.76	С
		C ILE A 487	49.755 54.772 56.749 1.00 44.95	С
		O ILE A 487	49.848 54.748 55.533 1.00 41.29	0
		CB ILE A 487	47.760 53.764 57.879 1.00 45.98	C
		CG1 ILE A 487	47.046 52.483 58.286 1.00 42.68	C
		CG2 ILE A 487	47.016 54.425 56.725 1.00 48.28	Ċ
		CD1 ILE A 487	47.114 51.396 57.264 1.00 43.54	Ċ
		N HIS A 488	50.166 55.842 57.432 1.00 48.83	N

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ATOM		50.832 56.961 56.775 1.00 49.75	С
ATOM	1384 C HIS A 488	52.052 56.545 55.987 1.00 48.04	С
ATOM	1385 O HIS A 488		Ο
ATOM	1386 CB HIS A 488	51.218 57.976 57.860 1.00 52.56	С
ATOM	1387 CG HIS A 488	51.999 59.098 57.240 1.00 57.68	С
ATOM	1388 ND1 HIS A 488	53.327 58.970 56.882 1.00 59.10	N
ATOM	1389 CD2 HIS A 488	51.620 60.355 56.920 1.00 59.02	С
ATOM	1390 CE1 HIS A 488	53.745 60.115 56.366 1.00 59.80	С
ATOM	1391 NE2 HIS A 488	52.734 60.958 56.385 1.00 60.71	N
ATOM	1392 N LEU A 489	52.888 55.639 56.452 1.00 46.72	N
ATOM	1393 CA LEU A 489		C
ATOM	1394 C LEU A 489		C
ATOM	1395 O LEU A 489		0
ATOM	1396 CB LEU A 489		C
ATOM	1397 CG LEU A 489		C
	1398 CD1 LEU A 489		C
	1399 CD2 LEU A 489		C
ATOM	1400 N MET A 490		N
ATOM	1401 CA MET A 490		C
ATOM	1402 C MET A 490		C
ATOM	1403 O MET A 490		0
ATOM	1404 CB MET A 490		C
ATOM	1405 CG MET A 490		C
	1406 SD MET A 490		S
	1407 CE MET A 490		C
	1408 N ALA A 491	50.596 54.711 52.631 1.00 50.20	N
ATOM	1409 CA ALA A 491	49.971 55.677 51.736 1.00 52.27	C
ATOM	1410 C ALA A 491	51.094 56.449 51.046 1.00 57.27	C
ATOM	1411 O ALA A 491		O C
	1412 CB ALA A 491	49.144 56.667 52.566 1.00 50.19	N
	1413 N LYS A 492	51.947 57.103 51.868 1.00 60.59	Ċ
	1414 CA LYS A 492		c
_	1415 C LYS A 492		_
	1416 O LYS A 492	54.478 57.443 49.416 1.00 63.72 53.920 58.444 52.351 1.00 63.55	OC
	1417 CB LYS A 492 1418 CG LYS A 492	54.888 59.509 51.953 1.00 65.38	C
	1422 N ALA A 493	53.818 55.599 50.461 1.00 59.10	N
	1423 CA ALA A 493		C
	1424 C ALA A 493	53.686 54.393 48.342 1.00 61.29	c
	1424 C ALA A 493	54.118 53.636 47.472 1.00 60.89	ŏ
	1426 CB ALA A 493	54.964 53.443 50.284 1.00 58.60	C
	1427 N GLY A 494	52.464 54.897 48.330 1.00 61.59	N
	1428 CA GLY A 494		Ċ
	1429 C GLY A 494	50.555 53.594 47.368 1.00 65.33	c
	1430 O GLY A 494	49.742 53.336 46.450 1.00 68.41	ŏ
	1431 N LEU A 495	50.533 52.861 48.493 1.00 63.96	N
	1431 N LEU A 495		C
	1432 CA LEU A 495	48.134 52.271 48.443 1.00 58.06	c
ATOM		47.735 53.379 48.799 1.00 56.91	Ö
AT OIM	1434 O LEO M433	77,733 33,373 70,733 1,00 50,71	_

49.732 51.021 49.907 1.00 58.36 С ATOM 1435 CB LEU A 495 C 50.979 50.136 50.029 1.00 57.55 ATOM 1436 CG LEU A 495 C 50.646 48.750 50.538 1.00 52.48 ATOM 1437 CD1 LEU A 495 C ATOM 1438 CD2 LEU A 495 51.767 50.006 48.718 1.00 58.19 47.275 51.380 47.919 1.00 58.45 N ATOM 1439 N THR A 496 45.857 51.787 47.808 1.00 57.29 C ATOM 1440 CA THR A 496 45.259 51.746 49.201 1.00 55.11 C ATOM 1441 C THR A 496 45.842 51.087 50.052 1.00 57.18 ATOM 1442 O THR A 496 0 45.038 50.909 46.867 1.00 57.90 C ATOM 1443 CB THR A 496 44.908 49.584 47.382 1.00 59.37 0 ATOM 1444 OG1 THR A 496 45.608 50.827 45.465 1.00 55.46 ATOM 1445 CG2 THR A 496 C ATOM 1446 N LEU A 497 44.128 52.356 49.468 1.00 55.27 N ATOM 1447 CA LEU A 497 43.533 52.264 50.784 1.00 57.86 C ATOM 1448 C LEU A 497 43.296 50.776 51.100 1.00 58.92 C ATOM 1449 O LEU A 497 43.492 50.361 52.231 1.00 61.57 0 ATOM 1450 CB LEU A 497 42.210 52.946 50.981 1.00 58.80 C C ATOM 1451 CG LEU A 497 42.176 54.431 51.253 1.00 62.15 C 40.717 54.877 51.444 1.00 65.00 ATOM 1452 CD1 LEU A 497 C ATOM 1453 CD2 LEU A 497 42.982 54.819 52.483 1.00 64.40 42.840 50.016 50.116 1.00 57.38 N ATOM 1454 N GLN A 498 ATOM 1455 CA GLN A 498 42.669 48.597 50.349 1.00 55.74 C C ATOM 1456 C GLN A 498 44.011 47.986 50.680 1.00 55.51 0 ATOM 1457 O GLN A 498 44.127 47.270 51.653 1.00 55.98 C 42.037 47.885 49.161 1.00 56.58 ATOM 1458 CB GLN A 498 41.901 46.397 49.303 1.00 58.82 ATOM 1459 CG GLN A 498 41.090 45.718 48.242 1.00 60.96 ATOM 1460 CD GLN A 498 41.304 45.928 47.056 1.00 63.68 0 ATOM 1461 OE1 GLN A 498 ATOM 1462 NE2 GLN A 498 40.134 44.875 48.625 1.00 62.29 N 45.055 48.224 49.917 1.00 56.42 N ATOM 1463 N GLN A 499 ATOM 1464 CA GLN A 499 46.365 47.642 50.216 1.00 56.77 C C 46.910 48.083 51.571 1.00 54.48 ATOM 1465 C GLN A 499 47.614 47.301 52.223 1.00 52.93 0 ATOM 1466 O GLN A 499 C ATOM 1467 CB GLN A 499 47.323 48.036 49.117 1.00 60.49 46.899 47.577 47.720 1.00 63.18 ATOM 1468 CG GLN A 499 C 47.943 48.181 46.768 1.00 66.27 ATOM 1469 CD GLN A 499 48.011 49.401 46.687 1.00 64.80 0 ATOM 1470 OE1 GLN A 499 48.689 47.282 46.139 1.00 67.90 N ATOM 1471 NE2 GLN A 499 ATOM 1472 N GLN A 500 46.626 49.298 51.982 1.00 49.56 N C ATOM 1473 CA GLN A 500 46.992 49.791 53.283 1.00 47.83 46.508 48.888 54.400 1.00 48.48 C ATOM 1474 C GLN A 500 ATOM 1475 O GLN A 500 47.258 48.320 55.208 1.00 49.65 0 C 46.422 51.236 53.446 1.00 46.97 ATOM 1476 CB GLN A 500 ATOM 1477 CG GLN A 500 47.355 52.289 52.796 1.00 42.84 46.661 53.575 52.477 1.00 39.88 C ATOM 1478 CD GLN A 500 45.984 54.134 53.307 1.00 38.64 0 ATOM 1479 OE1 GLN A 500 46.773 54.116 51.276 1.00 39.86 N ATOM 1480 NE2 GLN A 500 45,190 48,672 54,480 1.00 47.29 N ATOM 1481 N HIS A 501 C ATOM 1482 CA HIS A 501 44.552 47.861 55.505 1.00 42.58 C 44.996 46.422 55.449 1.00 43.22 ATOM 1483 C HIS A 501

A TO \ (1 40 4	O HIS A 501	45.204 45.723 56.460 1.00 45.13	0
ATOM		CB HIS A 501		Č
ATOM		CG AHIS A 501	42.245 47.480 54.393 0.50 43.18	C
ATOM ATOM		CG BHIS A 501	42.483 49.360 55.390 0.50 43.53	Č
		ND1AHIS A 501	41.395 48.280 53.648 0.50 44.55	N
ATOM		ND1BHIS A 501	42.849 50.353 56.286 0.50 45.90	N
ATOM		CD2AHIS A 501	42.076 46.219 53.916 0.50 43.33	C
ATOM		CD2BHIS A 501	41.577 49.916 54.558 0.50 42.37	č
ATOM		CE1AHIS A 501	40.760 47.503 52.765 0.50 44.96	č
ATOM	_	CEIBHIS A 501	42.205 51.471 55.986 0.50 46.12	Č
ATOM		NE2AHIS A 501	41.192 46.251 52.879 0.50 41.39	N
ATOM		NE2BHIS A 501	41.427 51.225 54.935 0.50 44.23	N
ATOM		N GLN A 502	45,258 45,931 54,236 1.00 42.10	N
ATOM	_	CA GLN A 502	45.665 44.544 54.122 1.00 40.55	Ċ
ATOM			47.070 44.369 54.674 1.00 41.26	c
ATOM			47.223 43.325 55.308 1.00 39.67	ŏ
ATOM		O GLN A 502 CB GLN A 502	45.696 44.016 52.715 1.00 41.12	c
ATOM		CG GLN A 502	44.574 44.566 51.860 1.00 40.32	Č
ATOM			44.320 43.508 50.808 1.00 42.78	č
ATOM		CD GLN A 502	43.242 42.927 50.851 1.00 49.36	Ö
ATOM		OE1 GLN A 502	45.312 43.328 49.986 1.00 41.14	N
ATOM		NE2 GLN A 502	47.950 45.305 54.294 1.00 40.71	N
ATOM		N ARG A 503	49.327 45.244 54.774 1.00 37.17	C
ATOM		CA ARG A 503	49.327 45.244 54.774 1.00 37.17	c
ATOM		C ARG A 503	49.915 44.683 57.058 1.00 33.57	Ö
ATOM		O ARG A 503 CB ARG A 503	50.177 46.335 54.137 1.00 40.97	C
ATOM		CG ARG A 503	51.671 46.162 54.431 1.00 45.67	Č
ATOM		CD ARG A 503	52.568 47.135 53.682 1.00 43.81	Č
ATOM		NE ARG A 503	53.964 46.879 53.959 1.00 40.13	N
ATOM		CZ ARG A 503	54.707 45.888 53.566 1.00 40.13	C
ATOM		NH1 ARG A 503		N
ATOM		NH2 ARG A 503		N
		N LEU A 504	48,556 46.448 56.780 1.00 33.53	N
		CA LEU A 504	48.500 46.664 58.228 1.00 34.14	C
		C LEU A 504	48.137 45.336 58.897 1.00 35.62	C
ATOM		O LEU A 504	48.825 44.902 59.816 1.00 38.42	Ö
		CB LEU A 504	47.501 47.693 58.699 1.00 33.74	C
		CG LEU A 504	47.267 47.904 60.186 1.00 32.73	Č
		CD1 LEU A 504		C
ATOM		CD2 LEU A 504	46.035 48.786 60.445 1.00 28.14	Č
ATOM ATOM		N ALA A 505	47.091 44.663 58.408 1.00 34.89	N
		CA ALA A 505	46.765 43.384 59.027 1.00 30.63	C
ATOM ATOM		C ALA A 505	47.844 42.353 58.814 1.00 30.88	c
			48.122 41.505 59.677 1.00 29.79	ŏ
ATOM		CB ALA A 505	45.417 42.908 58.511 1.00 32.54	C
ATOM		N GLN A 506	48.524 42.304 57.679 1.00 34.12	N
ATOM ATOM		CA GLN A 506	49.518 41.245 57.498 1.00 38.19	C
ATOM			50.601 41.441 58.544 1.00 36.89	c
			51.080 40.450 59.135 1.00 36.61	Ŏ
ATOM	1 232	O GLIAN 300	J1.000 T0.TJ0 J7.1JJ 1.00 J0.01	

C ATOM 1533 CB GLN A 506 50.040 41.099 56.070 1.00 45.24 C ATOM 1534 CG GLN A 506 48.933 40.987 55.024 1.00 53.31 C 49.221 41.548 53.640 1.00 56.75 ATOM 1535 CD GLN A 506 0 50.344 41.868 53.225 1.00 58.50 ATOM 1536 OE1 GLN A 506 N 48.166 41.687 52.827 1.00 57.68 ATOM 1537 NE2 GLN A 506 ATOM 1538 N LEU A 507 50.926 42.703 58.807 1.00 35.11 N C ATOM 1539 CA LEU A 507 51.952 42.976 59.826 1.00 32.90 C ATOM 1540 C LEU A 507 51.478 42.609 61.209 1.00 32.31 ATOM 1541 O LEU A 507 0 52.136 41.729 61.799 1.00 32.90 52.368 44.441 59.738 1.00 33.00 C ATOM 1542 CB LEU A 507 C ATOM 1543 CG LEU A 507 53.124 44.781 58.436 1.00 30.90 C ATOM 1544 CD1 LEU A 507 53,407 46,266 58,363 1.00 33,64 C 54.326 43.898 58.353 1.00 26.56 ATOM 1545 CD2 LEU A 507 ATOM 1546 N LEU A 508 50.381 43.190 61.720 1.00 29.06 N C ATOM 1547 CA LEU A 508 49.943 42.806 63.067 1.00 29.08 ATOM 1548 C LEU A 508 49.768 41.341 63.326 1.00 31.97 C 50.337 40.833 64.325 1.00 31.14 O ATOM 1549 O LEU A 508 C 48.726, 43.606 63.452 1.00 29.57 ATOM 1550 CB LEU A 508 C ATOM 1551 CG LEU A 508 48.966 45.119 63.181 1.00 30.98 C ATOM 1552 CD1 LEU A 508 47,708 45,877 63,540 1,00 28,17 C ATOM 1553 CD2 LEU A 508 50.185 45.594 63.945 1.00 25.29 49.333 40.542 62.333 1.00 31.90 N ATOM 1554 N LEU A 509 49.247 39.089 62.497 1.00 27.26 C ATOM 1555 CA LEU A 509 C 50.588 38.474 62.724 1.00 28.18 ATOM 1556 C LEU A 509 0 50.694 37.425 63.363 1.00 31.85 ATOM 1557 O LEU A 509 48.561 38.422 61.318 1.00 23.15 C ATOM 1558 CB LEU A 509 47.064 38.638 61.213 1.00 25.76 C ATOM 1559 CG LEU A 509 ATOM 1560 CD1 LEU A 509 46.469 37.882 60.057 1.00 24.02 C C 46.383 38.201 62.553 1.00 22.70 ATOM 1561 CD2 LEU A 509 ATOM 1562 N ILE A 510 N 51.638 39.130 62.234 1.00 31.59 C ATOM 1563 CA ILE A 510 52,997 38,574 62,437 1.00 31.40 C 53,334 38,772 63,913 1.00 30.63 ATOM 1564 C ILE A 510 0 ATOM 1565 O ILE A 510 54,010 37,877 64,420 1.00 31.28 C 54.010 39.169 61.483 1.00 34.47 ATOM 1566 CB ILE A 510 ATOM 1567 CG1 ILE A 510 53.979 38.367 60.163 1.00 37.44 C C ATOM 1568 CG2 ILE A 510 55.464 39.221 61.979 1.00 36.20 C ATOM 1569 CD1 ILE A 510 54.284 39.292 58.957 1.00 38.44 N ATOM 1570 N LEU A 511 52.783 39.785 64.592 1.00 27.44 C 53.047 39.907 66.021 1.00 28.51 ATOM 1571 CA LEU A 511 C ATOM 1572 C LEU A 511 52,535 38,703 66,757 1.00 32.18 53.240 38.241 67.686 1.00 38.66 0 ATOM 1573 O LEU A 511 ATOM 1574 CB LEU A 511 52.586 41.207 66.631 1.00 27.31 C C ATOM 1575 CG LEU A 511 53.002 42.452 65.796 1.00 28.29 52.496 43.707 66.420 1.00 24.10 C ATOM 1576 CD1 LEU A 511 54.528 42.469 65.580 1.00 24.27 C ATOM 1577 CD2 LEU A 511 51.468 38.078 66.371 1.00 34.01 N ATOM 1578 N SER A 512 C ATOM 1579 CA SER A 512 50.960 36.841 66.927 1.00 34.05 C ATOM 1580 C SER A 512 51.986 35.743 66.920 1.00 32.61 0 52.133 35.062 67.931 1.00 36.28 ATOM 1581 O SER A 512

		031-	_
ATOM	1582 CB SER A 512	49.730 36.415 66.073 1.00 36.45	C
ATOM	1583 OG SER A 512	48.657 36.567 67.007 1.00 41.54	.0
ATOM	1584 N HIS A 513	52.716 35.584 65.839 1.00 3 2.89	N
ATOM	1585 CA HIS A 513	53,766 34,577 65,746 1.00 33.89	С
ATOM	1586 C HIS A 513	54.969 34.971 66.579 1.00 33.11	С
ATOM	1587 O HIS A 513	55.588 34.159 67.263 1.00 34.48	0
ATOM		54.201 34.456 64.285 1.00 37.72	C
ATOM		53.098 34.018 63.383 1.00 40.23	С
ATOM	1590 ND1 HIS A 513	52.317 32.930 63.699 1.00 45.67	N
ATOM	1591 CD2 HIS A 513	52.646 34.429 62.190 1.00 43.55	С
ATOM	1592 CE1 HIS A 513	51.403 32.727 62.765 1.00 44.13	С
ATOM	1593 NE2 HIS A 513	51.605 33.640 61.829 1.00 44.41	N
ATOM	1594 N ILE A 514	55.288 36.268 66.530 1.00 33.10	N
ATOM	1595 CA ILE A 514	56.433 36.756 67.334 1.00 31.94	С
ATOM	1596 C ILE A 514	56.104 36.408 68.766 1.00 32.61	С
ATOM	1597 O ILE A 514	56.828 35.680 69.447 1.00 31.73	Ο
ATOM	1598 CB ILE A 514	56.732 38.208 66.994 1.00 30.68	С
ATOM	1599 CG1 ILE A 514	57.427 38.276 65.644 1.00 32.27	С
ATOM	1600 CG2 ILE A 514	57.654 38.845 68.035 1.00 32.24	С
ATOM	1601 CD1 ILE A 514	57.666 39.646 65.073 1.00 31.53	С
ATOM	1602 N ARG A 515	54.915 36.824 69.255 1.00 33.02	N
ATOM	1603 CA ARG A 515	54.554 36.406 70.609 1.00 32.91	С
	1604 C ARG A 515		C
ATOM		55.158 34.423 71.871 1.00 30.76	0
ATOM	1606 CB ARG A 515	53.047 36.671 70.737 1.00 36.94	С
ATOM	1607 CG ARG A 515	52.620 36.398 72.202 1.00 34.83	С
ATOM	1608 CD ARG A 515	53.103 37.571 72.993 1.00 33.43	С
ATOM			N
ATOM			С
ATOM	1611 NH1 ARG A 51	5 51.830 39.947 73.130 1.00 44.71	N
ATOM	1612 NH2 ARG A 51	5 50.638 39.215 74.964 1.00 46.87	N
ATOM	1613 N HIS A 516	54.238 34.150 69.837 1.00 36.19	N
ATOM		54.282 32.686 69.913 1.00 36.21	С
	1615 C HIS A 516	55.707 32.263 70.118 1.00 35.50	С
ATOM	1616 O HIS A 516	55.992 31.511 71.047 1.00 38.53	0
ATOM	1617 CB HIS A 516	53.671 32.077 68.655 1.00 39.92	С
ATOM	1618 CG HIS A 516	53.546 30.583 68.789 1.00 43.85	С
ATOM	1619 ND1 HIS A 516	52.560 30.007 69.565 1.00 45.49	N
ATOM	1620 CD2 HIS A 516	54.254 29.565 68.272 1.00 43.36	С
ATOM	1621 CE1 HIS A 516	52.671 28.702 69.525 1.00 42.83	С
ATOM	1622 NE2 HIS A 516	53.682 28.417 68.754 1.00 44.73	N
ATOM	1623 N MET A 517	56.642 32.758 69.280 1.00 34.02	N
ATOM	1624 CA MET A 517	58.044 32.363 69.496 1.00 33.79	С
	1625 C MET A 517	58.582 32.756 70.860 1.00 33.49	С
ATOM		59.128 31.928 71.588 1.00 35.14	0
ATOM		58.907 32.894 68.379 1.00 33.68	C
ATOM		7 58.635 32.256 67.047 1.00 34.56	С
ATOM		59.379 33.052 65.684 1.00 39.78	S
	1630 CE MET A 517	58.650 34.676 65.728 1.00 36.45	С

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ATOM 1631 N SER A 518 58.287 33.932 71.391 1.00 32.17 N C 58.814 34.255 72.728 1.00 33.21 ATOM 1632 CA SER A 518 ATOM 1633 C SER A 518 58.258 33.351 73.810 1.00 34.37 ATOM 1634 O SER A 518 59.026 32.919 74.699 1.00 30.18 O C ATOM 1635 CB SER A 518 58,660 35,740 73,023 1,00 31,26 ATOM 1636 OG SER A 518 58,344 35,917 74,367 1,00 28,79 0 56.954 33.031 73.778 1.00 32.58 N ATOM 1637 N ASN A 519 C ATOM 1638 CA ASN A 519 56.470 32.071 74.778 1.00 33.07 C ATOM 1639 C ASN A 519 57.147 30.732 74.586 1.00 37.75 ATOM 1640 O ASN A 519 57.570 30.029 75.506 1.00 35.09 0 ATOM 1641 CB ASN A 519 C 54.992 31.804 74.532 1.00 34.03 ATOM 1642 CG ASN A 519 54.162 33.022 74.946 1.00 32.85 54.541 33.610 75.938 1.00 29.80 0 ATOM 1643 OD1 ASN A 519 ATOM 1644 ND2 ASN A 519 53.088 33.307 74.226 1.00 33.79 N ATOM 1645 N LYS A 520 57.315 30.322 73.285 1.00 41.23 N 57.986 28.990 73.213 1.00 44.55 ATOM 1646 CA LYS A 520 C ATOM 1647 C LYS A 520 59.387 29.139 73.775 1.00 46.06 C ATOM 1648 O LYS A 520 59.917 28.260 74.463 1.00 49.52 0 ATOM 1649 CB LYS A 520 57.968 28.446 71.812 1.00 47.67 C 56.670 27.855 71.277 1.00 49.96 C ATOM 1650 CG LYS A 520 ATOM 1651 CD LYS A 520 55.721 27.402 72.365 1.00 52.10 C C ATOM 1652 CE LYS A 520 55.319 25.943 72.184 1.00 56.23 ATOM 1653 NZ LYS A 520 55.534 25.198 73.469 1.00 59.42 N 60.058 30.267 73.515 1.00 41.38 N ATOM 1654 N GLY A 521 C ATOM 1655 CA GLY A 521 61.432 30.412 73.867 1.00 39.78 ATOM 1656 C GLY A 521 61.658 30.534 75.347 1.00 40.02 C ATOM 1657 O GLY A 521 62.701 30.165 75.890 1.00 41.28 0 ATOM 1658 N MET A 522 60.678 31.118 75.998 1.00 41.42 N C ATOM 1659 CA MET A 522 60.768 31.349 77.433 1.00 42.08 ATOM 1660 C MET A 522 60.717 30.041 78.162 1.00 49.07 C ATOM 1661 O MET A 522 61.509 29.838 79.085 1.00 56.07 0 ATOM 1662 CB MET A 522 59.684 32.291 77.829 1.00 39.53 ATOM 1663 CG MET A 522 60.157 33.731 77.541 1.00 42.45 C ATOM 1664 SD MET A 522 59.509 34.694 78.912 1.00 49.75 S 58.965 36.121 77.995 1.00 43.03 C ATOM 1665 CE MET A 522 ATOM 1666 N GLU A 523 59.893 29.147 77.687 1.00 54.39 N C ATOM 1667 CA GLU A 523 59.767 27.782 78.081 1.00 58.80 ATOM 1668 C GLU A 523 61.095 27.061 77.843 1.00 60.25 C ATOM 1669 O GLU A 523 61.546 26.303 78.661 1.00 61.66 0 ATOM 1670 CB GLU A 523 58.760 27.032 77.156 1.00 60.53 C ATOM 1671 CG GLU A 523 57.490 26.591 77.833 1.00 65.10 ATOM 1672 CD GLU A 523 56.457 26.095 76.829 1.00 70.51 ATOM 1673 OE1 GLU A 523 56.619 24,909 76.435 1.00 72.53 0 55.526 26.874 76.438 1.00 69.51 ATOM 1674 OE2 GLU A 523 0 ATOM 1675 N HIS A 524 61.659 27.262 76.658 1.00 64.23 N ATOM 1676 CA HIS A 524 62.914 26.551 76.369 1.00 68.36 C ATOM 1677 C HIS A 524 64.007 27.149 77.237 1.00 68.67 C 64.733 26.419 77.903 1.00 66.17 ATOM 1678 O HIS A 524 0 ATOM 1679 CB HIS A 524 63.178 26.544 74.894 1.00 71.77 C

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ATOM	1680 CG HIS A 524	64.579 26.275 74.474 1.00 76.25	С
ATOM	1681 ND1 HIS A 524	65.129 26.831 73.329 1.00 77.80	N
ATOM		65.544 25.505 75.037 1.00 78.01	С
ATOM	1683 CE1 HIS A 524		С
	1684 NE2 HIS A 524	66.650 25.604 74.228 1.00 80.79	N
ATOM	1685 N LEU A 525	64.000 28.462 77.419 1.00 69.72	N
ATOM	1686 CA LEU A 525	64.976 29.072 78.309 1.00 73.19	C
		64.853 28.613 79.748 1.00 78.52	С
ATOM		65,872 28,438 80,422 1.00 78.86	0
ATOM	1689 CB LEU A 525	64.874 30.586 78.208 1.00 69.41	С
ATOM		66.064 31.385 77.682 1.00 65.43	C
ATOM		66.814 30.680 76.575 1.00 62.25	С
		65,590 32,752 77,232 1,00 63,11	С
	1693 N TYR A 526	63.651 28.440 80.291 1.00 85.31	N
ATOM		63.483 28.045 81.682 1.00 90.81	С
		63.638 26.558 81.891 1.00 91.90	С
		64.032 26.161 82.998 1.00 92.38	Ο
ATOM		62.194 28.564 82.270 1.00 97.06	С
ATOM		62.120 30.071 82.388 1.00104.66	С
ATOM		63.144 30.909 81.961 1.00106.68	C
		60.990 30.678 82.945 1.00107.36	C
ATOM		63.055 32.271 82.078 1.00108.14	С
		60.893 32.052 83.067 1.00109.12	·C
		61.937 32.845 82.629 1.00109.89	С
		61.841 34.218 82.752 1.00111.92	O
ATOM		63.511 25.754 80.846 1.00 92.46	N
ATOM	1706 CA SER A 527	63.790 24.328 80.992 1.00 95.45	С
ATOM	1707 C SER A 527	65.289 24.118 81.235 1.00 99.20	С
ATOM		65.687 23.257 82.013 1.00100.79	Ο
		63.296 23.511 79.819 1.00 93.04	C
		63.891 23.821 78.591 1.00 90.22	Ο
		66.130 24.898 80.579 1.00102.07	N
ATOM		67.568 24.846 80.673 1.00102.85	С
	1713 C MET A 528	68.047 25.302 82.050 1.00105.63	C
ATOM		68.088 24.486 82.976 1.00108.44	Ο
	1715 CB MET A 528	68.203 25.715 79.584 1.00100.04	C
	1716 CG MET A 528	68.106 25.183 78.174 1.00 97.06	С
	1717 SD MET A 528	68.537 26.345 76.869 1.00 93.64	S
	1718 CE MET A 528	69.354 27.655 77.751 1.00 94.41	С
ATOM		63.567 37.472 88.984 1.00 87.02	N
ATOM		64.688 38.390 89.191 1.00 83.59	С
	1721 C PRO A 535	64.668 39.490 88.133 1.00 77.41	С
ATOM		64.982 40.657 88.436 1.00 76.08	Ο
ATOM		65.996 37.567 89.158 1.00 85.89	С
ATOM		65.508 36.152 89.030 1.00 87.24	С
	1725 CD PRO A 535	64.069 36.136 88.567 1.00 87.96	С
ATOM		64.112 39.148 86.959 1.00 68.79	N
ATOM		64.158 40.084 85.833 1.00 61.48	С
ATOM		63.555 41.427 86.201 1.00 56.92	C
			

ATOM	1729	O LEU A 536	64.072 42.485 85.817 1.00 51.92	0
ATOM	1730	CB LEU A 536	63.499 39.485 84.625 1.00 61.82	С
ATOM	1731	CG LEU A 536	63.456 40.289 83.359 1.00 61.94	С
ATOM		CD1 LEU A 536	64.733 41.039 83.096 1.00 66.59	С
ATOM		CD2 LEU A 536	63,167 39.343 82.203 1.00 65.06	С
ATOM		N TYR A 537	62,461 41,317 86,973 1,00 52.04	N
ATOM		CA TYR A 537	61.734 42.468 87.440 1.00 49.60	С
ATOM		C TYR A 537	62,672 43,440 88,136 1,00 52,75	С
ATOM	1737		62.753 44.649 87.884 1.00 46.82	0
ATOM		CB TYR A 537	· ·	С
ATOM		CG TYR A 537		С
ATOM			60.333 44.054 89.909 1.00 51.84	С
ATOM			58.668 43.647 88.318 1.00 53.37	С
ATOM		CE1 TYR A 537		С
ATOM			57.946 44.761 88.732 1.00 54.40	С
ATOM		CZ TYR A 537		С
ATOM		OH TYR A 537	57.796 46.659 90.174 1.00 60.33	0
ATOM		N ASP A 538	63.393 42.826 89.102 1.00 58.32	N
ATOM		CA ASP A 538	64,281 43.628 89.951 1.00 62.64	С
ATOM		C ASP A 538	65.375 44.203 89.079 1.00 61.73	С
ATOM			65,730 45,378 89,192 1,00 64,00	0
ATOM			64.775 42.811 91.106 1.00 70.68	С
ATOM			63.674 42.219 91.974 1.00 75.57	С
ATOM			62.509 42.664 91.885 1.00 75.31	0
ATOM		OD2 ASP A 538	64.007 41.294 92.777 1.00 78.95	0
ATOM		N LEU A 539	65.864 43.356 88.177 1.00 58.42	N
ATOM		CA LEU A 539	66,891 43.778 87.247 1.00 56.11	С
ATOM		C LEU A 539	66.464 44.977 86.424 1.00 55.33	С
ATOM		O LEU A 539	67.198 45.960 86.300 1.00 56.67	Ο
ATOM		CB LEU A 539	67.152 42.613 86.314 1.00 59.46	С
ATOM			68.591 42.098 86.337 1.00 63.12	С
			68.627 40.824 85.472 1.00 66.12	С
ATOM		CD2 LEU A 539	69.575 43.132 85.869 1.00 63.42	С
	1762	N LEU A 540	65,286 44,888 85,814 1,00 52,86	N
		CA LEU A 540	64.782 45.949 84.965 1.00 50.07	С
		C LEU A 540	64,505 47.193 85.780 1.00 50.03	С
		O LEU A 540	64.704 48.340 85.350 1.00 45.66	Ο
		CB LEU A 540	63.513 45.418 84.280 1.00 51.61	С
		CG LEU A 540	63.707 44.278 83,279 1.00 50.39	С
		CD1 LEU A 540	62.415 43.605 82.952 1.00 47.32	С
		CD2 LEU A 540	64,353 44.785 81.982 1.00 52.21	С
		N LEU A 541	64.026 46.945 87.007 1.00 52.25	N
		CA LEU A 541	63.724 48.073 87.898 1.00 56.18	С
		C LEU A 541	65.035 48.788 88.182 1.00 57.88	С
		O LEU A 541	65.174 50.004 88.001 1.00 58.33	0
		CB LEU A 541	63.083 47.605 89.201 1.00 59.40	С
		CG LEU A 541	62.606 48.642 90.209 1.00 59.00	C
		CD1 LEU A 541	62.558 50.048 89.660 1.00 60.26	C
		CD2 LEU A 541	61.208 48.296 90.704 1.00 58.85	С
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ATOM	1778	N GLU A 542	66.025 47.944 88.573 1.00 56.65	N
			67.343 48.545 88.816 1.00 57.17	С
			67.772 49.230 87.534 1.00 58.47	С
ATOM	1781	O GLU A 542	67.976 50.450 87.489 1.00 60.82	0
			68.331 47.543 89.336 1.00 56.35	С
			67.805 48.491 86.424 1.00 57.50	N
ATOM	1788	CA MET A 543	68.200 49.160 85.176 1.00 60.04	С
ATOM	1789	C MET A 543	67.372 50.368 84.796 1.00 59.48	С
ATOM	1790	O MET A 543	67.911 51.423 84.433 1.00 51.56	0
ATOM	1791	CB MET A 543	68.226 48.108 84.077 1.00 62.92	С
			69.541 47.326 84.027 1.00 65.16	С
ATOM	1793	SD MET A 543	69,416 46,065 82,729 1,00 65,51	S
ATOM	1794	CE MET A 543	68.490 44.802 83.540 1.00 63.57	С
ATOM	1795	N LEU A 544	66.019 50.253 84.860 1.00 61.14	N
			65.209 51.402 84.496 1.00 62.86	С
			65.454 52.572 85.437 1.00 68.07	С
			65.323 53.711 84.983 1.00 66.46	0
			63.749 51.090 84.425 1.00 61.05	С
			63.154 50.387 83.217 1.00 58.33	С
			61.836 49.732 83.583 1.00 54.05	С
ATOM	1802	CD2 LEU A 544	62.994 51.351 82.067 1.00 58.50	С
			65.666 52.308 86.735 1.00 75.95	N
			65.833 53.447 87.631 1.00 84.89	C
			67.189 54.101 87.404 1.00 87.87	C
ATOM	1806	O ASP A 545	67.231 55.336 87.351 1.00 88.95	Ō
ATOM			65.567 53.176 89.095 1.00 89.55	C
ATOM			64.831 54.302 89.816 1.00 92.87	Č
			64.559 55.367 89.211 1.00 93.84	O
			64.502 54.146 91.022 1.00 94.22	Ō
			68.241 53.319 87.265 1.00 91.11	N
			69.593 53.826 87.034 1.00 94.05	C
			69.635 54.811 85.873 1.00 95.87	C
		O ALA A 546		Ō
		CB ALA A 546	70.548 52.674 86.773 1.00 94.06	C ·
		N HIS A 547	69.124 54.397 84.727 1.00 97.69	N
			68.937 55.242 83.573 1.00 99.06	C
		C HIS A 547	68.772 56.714 83.958 1.00 98.07	C
		O HIS A 547	69.164 57.583 83.141 1.00 95.96	Ō
		CB HIS A 547	67.659 54.755 82.832 1.00100.43	C
		CG HIS A 547	67.688 55.178 81.391 1.00101.48	Č
		ND1 HIS A 547	66.758 56.004 80.799 1.00100.77	N
		CD2 HIS A 547	68.612 54.876 80.435 1.00101.27	C
		CE1 HIS A 547		č
				N
		NE2 HIS A 547	00.224 33.313 73.233 1.00100.01	14
TER 1		HIS A 547 27 C1 ACBM A 38	54.836 38.076 80.880 0.50 61.38	С
				c
		28 C1 BCBM A 38		C
		29 C2 ACBM A 38		c
HETAT	W 183	0 C2 BCBM A 38	54.097 38.891 79.955 0.50 57.13	C

		55.146 37.147 79.993 0.50 61.86	0
HETATM 1832	O1 BCBM A 381		Ο
HETATM 1833	O2 ACBM A 381		0
	O2 BCBM A 381	53.285 40.058 78.041 0.50 58.80	0
HETATM 1835	C1 RAL A 600	69.571 36.223 71.917 1.00 31.33	С
HETATM 1836	C2 RAL A 600	69.816 37.448 71.352 1.00 30.47	С
HETATM 1837	C3 RAL A 600	69.083 37.933 70.305 1.00 31.66	С
HETATM 1838	O3 RAL A 600	69.410 39.186 69.850 1.00 32.81	Ο
HETATM 1839	C4 RAL A 600	68.029 37.167 69.794 1.00 33.99	С
HETATM 1840	C5 RAL A 600	67.765 35.956 70.385 1.00 33.49	С
HETATM 1841	S6 RAL A 600	66.638 34.815 69.986 1.00 33.96	S
HETATM 1842	C7 RAL A 600	67.001 33.691 71.192 1.00 34.48	С
HETATM 1843	C8 RAL A 600	66.347 32.356 71.301 1.00 35.62	С
HETATM 1844	C9 RAL A 600	66.087 31.727 70.099 1.00 35.20	С
HETATM 1845	C10 RAL A 600	65.560 30.446 70.128 1.00 38.32	С
HETATM 1846	C11 RAL A 600	65.259 29.817 71.320 1.00 39.44	С
HETATM 1847	O11 RAL A 600	64.735 28.525 71.249 1.00 46.17	Ο
HETATM 1848	C12 RAL A 600	65.562 30.428 72.519 1.00 36.17	С
HETATM 1849	C13 RAL A 600	66.106 31.706 72.480 1.00 34.51	С
HETATM 1850	C14 RAL A 600	68.556 35.468 71.464 1.00 31.87	С
HETATM 1851	C15 RAL A 600	68.128 34.150 71.906 1.00 33.10	С
HETATM 1852	C16 RAL A 600	68.771 33.463 72.918 1.00 36.94	С
HETATM 1853	O16 RAL A 600	69.368 32.412 72.653 1.00 40.67	Ο
HETATM 1854	C17 RAL A 600	68,768 33,917 74,313 1,00 36,96	С
	C18 RAL A 600	69.621 33.351 75.239 1.00 34.73	С
	C19 RAL A 600	69.633 33.745 76.563 1.00 34.67	С
HETATM 1857	C20 RAL A 600	68,733 34,725 76,978 1.00 37.20	С
HETATM 1858	C21 RAL A 600	67.879 35.305 76.057 1.00 40.93	С
HETATM 1859	C22 RAL A 600	67.907 34.910 74.730 1.00 39.84	С
HETATM 1860	O23 RAL A 600	68.555 35.259 78.220 1.00 36.45	Ο
HETATM 1861	C24 RAL A 600	69.461 34.837 79.228 1.00 38.03	С
HETATM 1862	C25 RAL A 600	69.311 35.692 80.458 1.00 43.08	С
HETATM 1863	N26 RAL A 600	69.023 37.110 80.557 1.00 46.61	N
HETATM 1864	C27 RAL A 600	68.720 37.437 81.965 1.00 47.65	С
HETATM 1865	C28 RAL A 600	68.544 38.946 82.229 1.00 48.95	С
HETATM 1866	C29 RAL A 600	67.338 39.404 81.393 1.00 50.06	С
HETATM 1867	C30 RAL A 600	67.804 39.197 79.919 1.00 50.91	С
HETATM 1868	C31 RAL A 600	67.960 37.681 79.707 1.00 50.67	С
ATOM 1869 N	1 LEU B 306	36.674 30.066 44.727 1.00 91.06	N
ATOM 1870 C	CA LEUB 306	35.325 30.211 45.360 1.00 93.16	С
ATOM 1871 C	C LEU B 306	35.377 31.143 46.562 1.00 89.78	С
ATOM 1872 C	LEU B 306	34.800 32.241 46.512 1.00 87.52	0
ATOM 1873 (CB LEUB 306	34.709 28.870 45.748 1.00 97.18	С
ATOM 1874 (CG LEUB 306	33.305 28.821 46.303 1.00101.83	С
ATOM 1875 C		32.367 29.926 45.882 1.00102.32	С
ATOM 1876 C		32.733 27.433 46.075 1.00103.20	С
ATOM 1877 N	N ALA B 307	36.135 30.778 47.577 1.00 87.24	N
ATOM 1878 (CA ALAB 307	36.337 31.584 48.780 1.00 84.71	С
ATOM 1879 (C ALA B 307	36.798 33.005 48.496 1.00 81.15	С

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ATOM	1880	O ALA B 307	36.351 33.998 49.052 1.00 79.11	0
			37.375 30.869 49.647 1.00 84.65	C
		N LEUB 308		N
		CA LEU B 308	38.271 34.398 47.137 1.00 79.21	C
		C LEU B 308	37.313 35.245 46.327 1.00 76.88	c
ATOM		O LEU B 308		ŏ
		CB LEU B 308		Č
		CG LEU B 308		Č
		CD1 LEU B 308	41.773 33.104 46.143 1.00 80.23	C
		CD2 LEU B 308	41.238 34.558 48.122 1.00 78.18	č
		N SER B 309	36.187 34.682 45.937 1.00 74.71	N
		CA SER B 309	35.273 35.475 45.127 1.00 74.21	C
		C SER B 309	34.123 36.021 45.944 1.00 71.62	C
ATOM		O SER B 309		Ö
ATOM		CB SER B 309		C
ATOM			34.808 33.289 44.133 1.00 76.34	Ö
		N LEUB 310	34.013 35.699 47.224 1.00 66.47	N
		CA LEU B 310	32.894 36.171 48.028 1.00 62.19	C
		C LEUB 310		C
ATOM		O LEU B 310		Ō
			32.908 35.534 49.430 1.00 60.65	C
ATOM			32.788 34.024 49.475 1.00 58.76	C
ATOM			32.907 33.539 50.906 1.00 61.50	C
ATOM		CD2 LEU B 310	31.497 33.570 48.834 1.00 57.77	С
ATOM		N THR B 311		N
ATOM	1905	CA THR B 311	31.802 39.704 48.787 1.00 56.79	С
ATOM	1906	C THR B 311	32.008 39.830 50.298 1.00 55.01	С
ATOM	1907	O THR B 311	32.030 38.818 50.985 1.00 52.51	0
ATOM	1908	CB THR B 311	30.554 40.446 48.308 1.00 55.64	С
ATOM	1909	OG1 THR B 311	29.386 39.919 48.896 1.00 54.85	• 0
ATOM	1910	CG2 THR B 311	30.473 40.352 46.792 1.00 54.89	С
ATOM	1911	N ALA B 312	32.152 41.040 50.812 1.00 53.60	N
			32.287 41.245 52.256 1.00 49.90	С
			31.033 40.697 52.891 1.00 49.90	C ·
ATOM	1914	O ALA B 312	31.143 39.803 53.723 1.00 51.10	Ο
ATOM	1915	CB ALA B 312	32.495 42.684 52.645 1.00 45.67	С
		N ASP B 313	29.852 41.129 52.428 1.00 52.72	N
		CA ASP B 313	28.645 40.569 53.019 1.00 56.00	С
		C ASP B 313	28.443 39.070 52.837 1.00 54.55	С
		O ASP B 313		О
			27.355 41.243 52.657 1.00 56.17	C
			27.253 42.696 52.951 1.00 58.96	C
		OD1 ASP B 313	27.527 43.200 54.061 1.00 58.70	0
	1923		26.891 43.365 51.949 1.00 62.08	0
		N GLN B 314	28.978 38.417 51.824 1.00 54.51	N
		CA GLN B 314	28.733 36.979 51.697 1.00 56.64	C
		C GLN B 314	29.567 36.196 52.694 1.00 55.43	C
			29.141 35.222 53.305 1.00 57.31	0
ATOM	1928	CB GLN B 314	29.002 36.513 50.279 1.00 57.95	С

28.127 37.253 49.263 1.00 57.78 C ATOM 1929 CG GLN B 314 ATOM 1930 CD GLN B 314 28.553 36.909 47.852 1.00 58.32 0 29.718 36.910 47.470 1.00 57.50 ATOM 1931 OE1 GLN B 314 N ATOM 1932 NE2 GLN B 314 27.523 36.594 47.098 1.00 60.62 ATOM 1933 N MET B 315 30.754 36.685 52.891 1.00 52.23 N C ATOM 1934 CA MET B 315 31.739 36.241 53.827 1.00 49.70 ATOM 1935 C MET B 315 31.133 36.254 55.234 1.00 46.39 C 31.194 35.291 55.998 1.00 41.29 ATOM 1936 O MET B 315 0 ATOM 1937 CB MET B 315 32.848 37.320 53.756 1.00 52.35 33.985 37.099 54.749 1.00 54.04 ATOM 1938 CG MET B 315 C 35.044 35.772 54.203 1.00 56.39 ATOM 1939 SD MET B 315 34.543 34.408 55.191 1.00 56.31 C ATOM 1940 CE MET B 315 30.591 37.428 55.579 1.00 42.31 ATOM 1941 N VAL B 316 N C ATOM 1942 CA VAL B 316 29.993 37.536 56.893 1.00 42.79 ATOM 1943 C VAL B 316 28.882 36.517 57.087 1.00 41.54 C 28.898 35.860 58.125 1.00 43.23 ATOM 1944 O VAL B 316 0 C ATOM 1945 CB VAL B 316 29.401 38.908 57.216 1.00 41.66 C ATOM 1946 CG1 VAL B 316 28.789 38.844 58.592 1.00 41.71 ATOM 1947 CG2 VAL B 316 30.437 39.993 57.108 1.00 44.09 C 27.937 36.398 56.163 1.00 40.87 ATOM 1948 N SER B 317 N C ATOM 1949 CA SER B 317 26,845 35,448 56,455 1.00 44.95 27.340 34.030 56.379 1.00 42.50 C ATOM 1950 C SER B 317 26.880 33.149 57.086 1.00 42.42 ATOM 1951 O SER B 317 0 C ATOM 1952 CB SER B 317 25.636 35.630 55.554 1.00 46.95 ATOM 1953 OG SER B 317 26.099 35.778 54.245 1.00 51.75 0 28.324 33.767 55.504 1.00 40.11 ATOM 1954 N ALA B 318 N ATOM 1955 CA ALA B 318 28.795 32.377 55.488 1.00 38.46 C 29.217 32.030 56.928 1.00 40.51 C ATOM 1956 C ALA B 318 28.959 30.989 57.494 1.00 42.17 ATOM 1957 O ALA B 318 0 C ATOM 1958 CB ALA B 318 29,920 32,190 54,554 1.00 32,54 ATOM 1959 N LEUB 319 29.968 32.952 57.500 1.00 42.20 N C ATOM 1960 CA LEU B 319 30.565 32.839 58.786 1.00 39.71 29.546 32.729 59.904 1.00 40.27 C ATOM 1961 C LEUB 319 ATOM 1962 O LEUB 319 29.688 31.814 60.716 1.00 37.79 0 C 31.495 34.038 58.998 1.00 33.71 ATOM 1963 CB LEUB 319 ATOM 1964 CG LEU B 319 32.768 33.858 58.194 1.00 31.85 ATOM 1965 CD1 LEU B 319 33.727 35.029 58.472 1.00 33.62 33.378 32.498 58.401 1.00 26.82 C ATOM 1966 CD2 LEU B 319 ATOM 1967 N LEUB 320 28.591 33.630 59.877 1.00 41.15 N 27.523 33.694 60.871 1.00 41.53 C ATOM 1968 CA LEU B 320 ATOM 1969 C LEUB 320 26,745 32,394 60.833 1.00 45.93 C ATOM 1970 O LEUB 320 26.314 31.873 61.869 1.00 49.20 0 C ATOM 1971 CB LEUB 320 26.591 34.866 60.594 1.00 36.95 27.082 36.214 61.131 1.00 37.97 ATOM 1972 CG LEUB 320 ATOM 1973 CD1 LEU B 320 26.133 37.337 60.825 1.00 33.54 C ATOM 1974 CD2 LEU B 320 27.335 36.118 62.636 1.00 35.35 ATOM 1975 N ASP B 321 26.663 31.823 59.644 1.00 47.02 N ATOM 1976 CA ASP B 321 26.010 30.577 59.440 1.00 50.66 C ATOM 1977 C ASP B 321 26.740 29.406 60.030 1.00 46.60 C

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			26.147 28.446 60.485 1.00 51.45	0
ATOM			25.910 30.237 57.913 1.00 59.17	C
ATOM			24.471 29.735 57.741 1.00 63.60	C
ATOM			23.615 30.631 57.906 1.00 64.90	0
			24.323 28.523 57.513 1.00 66.90	0
		N ALAB 322		N
		CA ALAB 322		C
		C ALA B 322		C
		O ALA B 322		0
ATOM		CB ALAB 322	30.218 28.587 59.801 1.00 32.90	C
ATOM		N GLUB 323		N
ATOM			28.626 29.441 64.129 1.00 35.05	C
		C GLUB 323		C
		O GLU B 323		0
			27.842 30.599 64.703 1.00 32.26	C
			28.693 31.894 64.759 1.00 35.65	C
			29,907 31.568 65.638 1.00 37.28	C
ATOM			30.881 31.084 65.044 1.00 37.53	0
ATOM			29.839 31.721 66.859 1.00 37.73	0
ATOM			29.069 27.613 65.654 1.00 37.32	N
•-		CA PRO B 324		С
_		C PRO B 324		C
ATOM			27.445 27.974 67.725 1.00 35.69	0
ATOM			29.926 25.912 67.120 1.00 36.62	C
ATOM			30.795 27.125 67.154 1.00 35.28	C
ATOM			30.285 28.185 66.199 1.00 37.93	С
ATOM		N PRO B 325		N
ATOM		CA PROB 325		С
ATOM		C PRO B 325		C
ATOM		O PRO B 325		0
ATOM		CB PRO B 325		C
ATOM			26.275 23.689 68.477 1.00 30.29	C
ATOM			27.141 24.441 67.507 1.00 32.36	C
ATOM		N ILE B 326	25.929 27.031 71.231 1.00 35.84	N
		CA ILE B 326	26.567 27.139 72.555 1.00 36.70	С
		C ILE B 326	26.240 25.913 73.382 1.00 38.88	С
ATOM			25.058 25.724 73.698 1.00 42.79	0
		CB ILE B 326	26.123 28.433 73.253 1.00 37.21	С
		CG1 ILE B 326	26.777 29.593 72.434 1.00 35.81	C
		CG2 ILE B 326	26.616 28.473 74.693 1.00 32.67	C
		CD1 ILE B 326	26.211 30.920 72.862 1.00 41.70	C
		N LEUB 327	27.179 25.020 73.679 1.00 35.51	N
		CA LEUB 327	26.891 23.820 74.412 1.00 30.60	С
		C LEU B 327	26.734 24.065 75.899 1.00 35.93	C
		O LEU B 327	27.083 25.118 76.388 1.00 38.14	0
		CB LEUB 327	28.035 22.821 74.220 1.00 30.41	C
		CG LEUB 327		С
		CD1 LEU B 327		C
ATOM	2026	CD2 LEU B 327	27.149 22.038 71.986 1.00 33.00	С

ATOM	2027	N TYR B 328	26.248 23.082 76.662 1.00 38.95	N
ATOM	2028	CA TYR B 328	26.048 23.110 78.065 1.00 39.09	С
ATOM	2029	C TYR B 328	26.937 22.118 78.795 1.00 40.90	С
ATOM	2030	O TYR B 328	27.340 21.115 78.209 1.00 37.06	0
ATOM	2031	CB TYR B 328	24.637 22.721 78.470 1.00 43.01	С
ATOM	2032	CG TYR B 328	23.637 23.835 78.325 1.00 45.81	С
ATOM	2033	CD1 TYR B 328	23.193 24.252 77.073 1.00 43.80	С
ATOM	2034	CD2 TYR B 328	23.148 24.465 79.472 1.00 46.54	С
ATOM	2035	CE1 TYR B 328	22.264 25.251 76.964 1.00 44.96	С
ATOM	2036	CE2 TYR B 328	22.222 25.499 79.356 1.00 45.50	С
ATOM		CZ TYR B 328	21.799 25.880 78.103 1.00 46.55	С
ATOM		OH TYR B 328	20.868 26.894 77.991 1.00 48.51	Ο
ATOM	2039	N SER B 329	27.188 22.518 80.048 1.00 45.16	N
ATOM	2040	CA SER B 329		С
ATOM	2041		27.211 20.428 81.217 1.00 53.86	С
ATOM	2042		26.079 20.598 81.626 1.00 55.54	0
ATOM		CB SER B 329	28.437 22.309 82.217 1.00 47.00	С
ATOM	2044	OG SER B 329	29.422 21.345 82.720 1.00 47.21	0
ATOM	2045		27.732 19.283 81.042 1.00 59.98	N
ATOM		CA GLU B 330	26.998 18.042 81.324 1.00 70.19	С
ATOM		C GLU B 330	27.154 17.795 82.810 1.00 76.09	C
ATOM	2048		28.098 17.104 83.179 1.00 78.83	0
ATOM		CB GLUB 330		C
ATOM		CG GLU B 330		С
ATOM		CD GLUB 330		C
ATOM		OE1 GLU B 330	28.322 15.500 78.291 1.00 77.49	0
ATOM		OE2 GLU B 330	28.109 13.726 79.613 1.00 76.55	0
ATOM		N TYR B 331	26.292 18.399 83.607 1.00 83.66	N
ATOM		CA TYR B 331	26.452 18.272 85.060 1.00 91.44	C
ATOM	2056	=	25.131 18.314 85.781 1.00 92.28	C
ATOM	2057		25.037 18.634 86.965 1.00 93.86	0
ATOM			27.466 19.336 85.469 1.00 97.13	C
ATOM		CG TYR B 331	27.069 20.568 86.213 1.00101.71	C
		CD1 TYR B 331	26.608 21.704 85.561 1.00103.32	C
		CD2 TYR B 331	27.178 20.619 87.608 1.00104.18	C
		CE1 TYR B 331	26.226 22.828 86.263 1.00105.97	C
		CE2 TYR B 331	26.828 21.752 88.324 1.00106.55	C
		CZ TYR B 331	26.347 22.858 87.642 1.00107.31	C
ATOM		OH TYR B 331	25.995 24.000 88.323 1.00107.29	.0
		N ALAB340	39.286 16.946 89.923 1.00 93.98	N
		CA ALAB 340	38.917 16.738 88.521 1.00 93.62	C
		C ALA B 340	37.402 16.787 88.327 1.00 90.09	C
		O ALA B 340	36.868 16.237 87.370 1.00 90.38	0
		CB ALAB 340	39.519 15.472 87.926 1.00 94.53	C
		N SER B 341	36.706 17.458 89.239 1.00 85.89	N
		CA SER B 341	35.276 17.676 89.073 1.00 82.06	С
ATOM		C SER B 341	35.174 18.844 88.061 1.00 78.61	C
ATOM				0
ATOM	2075	CB SER B 341	34.610 18.188 90.341 1.00 83.38	С

ATOM	2076	OG SER B 341	35.256 19.414 90.728 1.00 85.02	Ο
ATOM	2077	N MET B 342	35.722 19.964 88.528 1.00 71.83	N
ATOM	2078	CA MET B 342	35.738 21.170 87.702 1.00 67.11	С
ATOM	2079	C MET B 342	36.582 20.918 86.469 1.00 62.56	С
ATOM	2080	O MET B 342	36.233 21.329 85.369 1.00 62.00	0
ATOM	2081	CB MET B 342	36.320 22.295 88.511 1.00 71.06	C
ATOM	2082	CG MET B 342	36.550 23.547 87.695 1.00 76.61	С
ATOM	2083	SD MET B 342	36.328 24.989 88.764 1.00 82.30	S
ATOM	2084	CE MET B 342	37.859 25.853 88.353 1.00 81.45	С
ATOM	2085	N MET B 343	37.682 20.186 86.669 1.00 58.18	N
ATOM	2086	CA MET B 343	38.521 19.887 85.520 1.00 57.17	С
ATOM	2087	C MET B 343	37.765 18.915 84.625 1.00 53.51	С
ATOM		O MET B 343	37.989 18.950 83.422 1.00 54.37	Ο
ATOM		CB MET B 343	39.915 19.428 85.885 1.00 60.29	С
ATOM			40.925 20.583 85.969 1.00 64.87	С
ATOM			40.885 21.649 84.487 1.00 70.97	S
ATOM		CE MET B 343	41.239 20.401 83.224 1.00 67.55	С
ATOM	2093		36.877 18.128 85.204 1.00 50.03	N
ATOM			36.100 17.109 84.489 1.00 45.01	С
ATOM		C GLY B 344	35.089 17.784 83.576 1.00 44.23	C
ATOM		O GLY B 344	35.007 17.591 82.362 1.00 44.89	0
ATOM		N LEUB 345	34.395 18.715 84.226 1.00 41.93	N
ATOM		CA LEU B 345	33.397 19.513 83.562 1.00 42.59	C
ATOM		C LEUB 345	33.964 20.248 82.346 1.00 43.04	C
		O LEUB 345	33.393 20.250 81.229 1.00 40.37	0
ATOM		CB LEUB 345	32.765 20.451 84.561 1.00 43.09	C
ATOM		CG LEUB 345		C
ATOM			30.750 21.109 85.884 1.00 42.87	C
		CD2 LEU B 345	30.825 18.815 84.964 1.00 43.41	C
		N LEUB 346	35.112 20.870 82.544 1.00 41.05	N C
		C LEUB 346	35.738 21.616 81.445 1.00 40.63 36.303 20.717 80.373 1.00 39.43	c
		O LEUB 346	36.259 21.034 79.158 1.00 38.60	Ö
		CB LEU B 346	36.802 22.539 82.083 1.00 40.84	C
		CG LEU B 346	36.140 23.535 83.040 1.00 40.19	C
		CD1 LEU B 346	37.202 24.319 83.759 1.00 40.76	Č
		CD2 LEU B 346	35.106 24.415 82.336 1.00 37.83	c
		N THR B 347	36,709 19.510 80.739 1.00 38.21	N
		CA THR B 347	37.285 18.607 79.711 1.00 38.77	C
		C THR B 347	36.175 18.060 78.878 1.00 39.07	C
ATOM			36.273 17.880 77.679 1.00 41.54	O
		CB THR B 347	38.055 17.505 80.445 1.00 35.92	C
		OG1 THR B 347	38.912 18.218 81.351 1.00 38.30	0
		CG2 THR B 347	38,918 16.662 79.577 1.00 35.35	С
		N ASN B 348	35.066 17.774 79.565 1.00 42.21	N
		CA ASN B 348	33.930 17.197 78.816 1.00 40.77	C
		C ASN B 348	33.447 18.316 77.893 1.00 37.78	С
ATOM			33.306 18.016 76.707 1.00 41.02	0
ATOM	2124	CB ASN B 348	32.835 16.674 79.718 1.00 46.33	С

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ATOM	2223 CG TRP B 360	33.266 27.248 62.885 1.00 31.31	C.
		32.726 28.432 62.489 1.00 30.14	С
ATOM	2225 CD2 TRP B 360	34.656 27.477 63.095 1.00 27.29	С
ATOM	2226 NE1 TRP B 360	33.690 29.405 62.477 1.00 28.74	N
	2227 CE2 TRP B 360		С
	2228 CE3 TRP B 360		С
	2229 CZ2 TRP B 360		С
	2230 CZ3 TRP B 360		С
		37.152 28.642 63.395 1.00 25.71	С
		34.937 24.709 61.298 1.00 39.67	N
ATOM	2233 CA ALAB 361	36.185 24.796 60.527 1.00 43.20	С
		35.935 24.626 59.036 1.00 42.09	C
		36.251 25.465 58.184 1.00 37.43	Ō
		37.143 23.729 61.106 1.00 42.72	Ċ
	2237 N LYS B 362	35.254 23.526 58.685 1.00 43.79	N
	2238 CA LYS B 362	34,880 23,171 57,339 1.00 44.31	C
			C
		33.967 24.256 55.448 1.00 46.74	Ō
		34.254 21.793 57.234 1.00 44.89	С
		35.116 20.662 57.747 1.00 47.52	C
		36.192 20.357 56.692 1.00 53.22	C
	2244 CE LYS B 362		С
		37.853 18.714 55.815 1.00 58.66	N
	2246 N ARG B 363		N
		32.688 26.238 56.688 1.00 46.46	С
		33.447 27.545 56.666 1.00 47.06	С
		32.952 28.594 56.190 1.00 47.77	0
		31.285 26.352 57.252 1.00 51.47	С
		30.599 24.978 57.257 1.00 57.74	С
ATOM			С
	2253 NE ARG B 363	_	N
	2254 CZ ARG B 363		С
	2255 NH1 ARG B 363		N
		27.503 23.448 60.423 1.00 78.39	N
	2257 N VAL B 364	34.701 27.524 57.115 1.00 43.37	N
	2258 CA VAL B 364	35.437 28.786 56.962 1.00 46.62	С
ATOM	2259 C VAL B 364	35.978 28.824 55.552 1.00 51.16	С
ATOM	2260 O VAL B 364	36.718 27.947 55.063 1.00 53.83	Ο
ATOM	2261 CB VAL B 364	36.455 28.883 58.101 1.00 45.62	С
ATOM	2262 CG1 VAL B 364	37.501 29.930 57.814 1.00 40.24	С
ATOM	2263 CG2 VAL B 364	35.697 29.179 59.395 1.00 41.67	С
ATOM	2264 N PRO B 365	35.581 29.804 54.781 1.00 54.29	N
ATOM	2265 CA PRO B 365	36.002 30.007 53.408 1.00 54.11	C
ATOM	2266 C PRO B 365	37.505 29.941 53.286 1.00 56.48	С
ATOM	2267 O PRO B 365	38.258 30.675 53.911 1.00 57.71	0
	2268 CB PRO B 365	35.484 31.391 52.999 1.00 55.74	С
	2269 CG PRO B 365	34.239 31.482 53.865 1.00 56.60	С
		34.660 30.870 55.221 1.00 57.46	С
ATOM	2271 N GLY B 366	37.968 28.989 52.492 1.00 59.01	N

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ATOM	2272 CA GLY B 366	39.367 28.719 52.206 1.00 56.53	С
ATOM	2273 C GLY B 366	39.814 27.449 52.896 1.00 56.39	С
ATOM	2274 O GLYB 366	40.701 26.721 52.453 1.00 57.87	Ο
ATOM	2275 N PHE B 367	39.185 27.178 54.044 1.00 54.29	N
ATOM	2276 CA PHE B 367	39.568 26.030 54.829 1.00 51.31	С
ATOM	2277 C PHE B 367	39.509 24.725 54.071 1.00 51.54	С
ATOM	2278 O PHE B 367	40.379 23.888 54.307 1.00 55.10	0
ATOM	2279 CB PHE B 367	38.689 25.855 56.102 1.00 45.65	С
ATOM	2280 CG PHE B 367	39.438 24.995 57.091 1.00 41.76	C
ATOM	2281 CD1 PHE B 367	40.589 25.494 57.707 1.00 40.04	С
ATOM	2282 CD2 PHE B 367	39.023 23.713 57.375 1.00 38.51	С
ATOM	2283 CE1 PHE B 367	41.273 24.731 58.636 1.00 37.07	С
ATOM	2284 CE2 PHE B 367	39.717 22.963 58.321 1.00 36.35	С
ATOM	2285 CZ PHE B 367	40.834 23.460 58.936 1.00 33.86	C
ATOM	2286 N VAL B 368	38.474 24.480 53.298 1.00 52.13	N
ATOM	2287 CA VAL B 368	38,363 23.114 52.736 1.00 54.30	С
ATOM	2288 C VAL B 368	39.143 22.975 51.486 1.00 57.80	С
ATOM	2289 O VAL B 368	39.401 21.869 50.998 1.00 63.60	Ο
ATOM	2290 CB VAL B 368	36.907 22.637 52.764 1.00 53.61	С
ATOM	2291 CG1 VAL B 368	36.182 22.937 51.495 1.00 47.24	С
ATOM	2292 CG2 VAL B 368	36.822 21.182 53.236 1.00 53.23	C
ATOM	2293 N ASP B 369	39.682 24.036 50.920 1.00 59.22	N
ATOM	2294 CA ASP B 369	40.571 24.101 49.792 1.00 59.42	C
ATOM	2295 C ASP B 369	41.975 23.618 50.187 1.00 61.08	C
ATOM	2296 O ASP B 369	42.917 23.513 49.408 1.00 65.57	0
ATOM	2297 CB ASP B 369	40.764 25.614 49.507 1.00 60.75	С
ATOM	2298 CG ASP B 369	39.544 26.116 48.756 1.00 62.62	С
ATOM	2299 OD1 ASP B 369	38.792 25.215 48.325 1.00 64.13	· O
ATOM	2300 OD2 ASP B 369	39.395 27.336 48.564 1.00 62.51	0
ATOM	2301 N LEUB 370	42.173 23.356 51.457 1.00 57.11	N
ATOM	2302 CA LEUB 370	43.421 22.936 51.990 1.00 56.49	С
ATOM	2303 C LEUB 370	43.455 21.412 52.023 1.00 57.13	С
ATOM	2304 O LEUB 370	42.388 20.842 52.060 1.00 59.40	0
ATOM	2305 CB LEUB 370	43.514 23.456 53.430 1.00 55.70	С
ATOM	2306 CG LEUB 370	43.789 24.926 53.676 1.00 52.48	С
ATOM	2307 CD1 LEUB 370	44.811 25.033 54.778 1.00 52.72	С
ATOM	2308 CD2 LEU B 370	44.290 25.641 52.439 1.00 54.40	С
ATOM	2309 N THR B 371	44.648 20.857 52.022 1.00 56.95	N
	2310 CA THR B 371	44.804 19.440 52.137 1.00 57.71	С
	2311 C THR B 371	44.344 19.082 53.556 1.00 58.84	С
ATOM	2312 O THR B 371	44.392 19.912 54.471 1.00 58.64	Ο
	2313 CB THR B 371	46.257 18.949 51.967 1.00 59.95	С
	2314 OG1 THR B 371	47.063 19.177 53.118 1.00 58.30	O
	2315 CG2 THR B 371	46.924 19.573 50.745 1.00 60.40	С
	2316 N LEUB 372	43.993 17.828 53.732 1.00 60.21	N
	2317 CA LEUB 372	43.598 17.318 55.034 1.00 62.03	C
	2318 C LEUB 372	44.728 17.567 56.026 1.00 63.78	С
ATOM	2319 O LEUB 372	44.474 18.069 57.134 1.00 66.06	0
ATOM	2320 CB LEUB 372	43.218 15.852 54.890 1.00 62.64	С

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42.780 15.076 56.117 1.00 66.44 C ATOM 2321 CG LEUB 372 C 41.896 15.921 57.053 1.00 64.82 ATOM 2322 CD1 LEU B 372 ATOM 2323 CD2 LEU B 372 42.018 13.815 55.715 1.00 67.73 C ATOM 2324 N HIS B 373 45.992 17.295 55.677 1.00 64.79 N 47.067 17.517 56.603 1.00 66.99 ATOM 2325 CA HIS B 373 C ATOM 2326 C HIS B 373 47.115 18.970 57.044 1.00 61.47 C ATOM 2327 O HIS B 373 47.443 19.187 58.196 1.00 59.54 0 ATOM 2328 CB HIS B 373 48.496 17.289 56.089 1.00 76.41 C ATOM 2329 CG HIS B 373 48.547 15.901 55.537 1.00 87.82 ATOM 2330 ND1 HIS B 373 47.917 14.825 56.131 1.00 89.75 ATOM 2331 CD2 HIS B 373 49.156 15.441 54.408 1.00 93.11 C ATOM 2332 CE1 HIS B 373 48.126 13.744 55.408 1.00 92.37 C ATOM 2333 NE2 HIS B 373 48.876 14.081 54.357 1.00 95.93 N ATOM 2334 N ASP B 374 46.952 19.840 56.063 1.00 55.09 N ATOM 2335 CA ASP B 374 46.990 21.246 56.394 1.00 53.61 C ATOM 2336 C ASP B 374 45.862 21.661 57.317 1.00 52.72 C ATOM 2337 O ASP B 374 46.101 22.487 58.199 1.00 52.25 0 ATOM 2338 CB ASP B 374 46.929 22.068 55.120 1.00 56.95 C ATOM 2339 CG ASP B 374 48.340 22.005 54.524 1.00 58.90 ATOM 2340 OD1 ASP B 374 49.234 21.611 55.307 1.00 59.70 ATOM 2341 OD2 ASP B 374 48.382 22.331 53.335 1.00 60.88 ATOM 2342 N GLN B 375 44.696 21.062 57.078 1.00 48.20 ATOM 2343 CA GLN B 375 43.547 21.361 57.929 1.00 44.27 C ATOM 2344 C GLN B 375 43.825 20.918 59.341 1.00 42.91 ATOM 2345 O GLN B 375 43.586 21.609 60.327 1.00 44.49 ATOM 2346 CB GLN B 375 42.329 20.689 57.324 1.00 43.58 C ATOM 2347 CG GLN B 375 41.962 21.403 55.992 1.00 42.71 ATOM 2348 CD GLN B 375 40.671 20.795 55.473 1.00 46.29 ATOM 2349 OE1 GLN B 375 40.180 19.789 55.992 1.00 46.02 ATOM 2350 NE2 GLN B 375 40.062 21.425 54.480 1.00 49.60 N ATOM 2351 N VAL B 376 44.428 19.771 59.518 1.00 42.38 N ATOM 2352 CA VAL B 376 44.734 19.265 60.872 1.00 41.31 C ATOM 2353 C VAL B 376 45.808 20.127 61.495 1.00 45.24 ATOM 2354 O VAL B 376 45.836 20.342 62.711 1.00 48.81 O ATOM 2355 CB VAL B 376 45.295 17.844 60.678 1.00 39.53 ATOM 2356 CG1 VAL B 376 45.791 17.269 61.958 1.00 37.82 ATOM 2357 CG2 VAL B 376 44.319 16.979 59.903 1.00 37.59 ATOM 2358 N HIS B 377 46.740 20,644 60.667 1.00 44.81 N 47.792 21.478 61.269 1.00 44.39 C ATOM 2359 CA HIS B 377 ATOM 2360 C HIS B 377 47.155 22.780 61.769 1.00 41.44 C 47.358 23.208 62.881 1.00 42.24 ATOM 2361 O HIS B 377 0 ATOM 2362 CB HIS B 377 48.970 21.761 60.372 1.00 41.82 C ATOM 2368 N LEUB 378 46.287 23.384 60.995 1.00 38.79 ATOM 2369 CA LEUB 378 45.586 24.560 61.452 1.00 37.49 C ATOM 2370 C LEU B 378 44.817 24.307 62.738 1.00 39.70 C ATOM 2371 O LEUB 378 44.965 25.065 63.742 1.00 40.23 0 ATOM 2372 CB LEUB 378 44.792 25.084 60.278 1.00 34.49 C ATOM 2373 CG LEUB 378 45.660 25.626 59.142 1.00 33.30 ATOM 2374 CD1 LEU B 378 44,776 26,268 58,061 1,00 35,31

ATOM		CD2 LEU B 378	46.652 26.648 59.629 1.00 31.86	С
ATOM		N LEUB 379	44.014 23.264 62.855 1.00 39.55	N
ATOM		CA LEUB 379	43.281 23.045 64.108 1.00 39.47	C
ATOM		C LEUB 379	44.236 22.621 65.183 1.00 40.67	C
ATOM		O LEUB 379	44.113 22.953 66.367 1.00 44.03	0
ATOM		CB LEUB 379	42.165 22.022 63.905 1.00 36.04	С
ATOM		CG LEU B 379	41.035 22.590 63.044 1.00 36.14	С
ATOM		CD1 LEU B 379	40.367 21.487 62.267 1.00 35.56	С
ATOM		CD2 LEU B 379	40.005 23.346 63.905 1.00 35.13	С
ATOM		N GLU B 380	45.299 21.916 64.808 1.00 44.30	N
ATOM		CA GLUB 380	46.131 21.413 65.904 1.00 47.28	С
ATOM	2386	C GLU B 380	46.648 22.562 66.732 1.00 46.23	С
ATOM	2387		46.674 22.437 67.945 1.00 47.50	0
		CB GLUB 380	47.223 20.484 65.491 1.00 55.36	C
		CG GLUB 380	47.687 19.578 66.656 1.00 62.14	С
		CD GLUB 380	48.998 18.908 66.279 1.00 68.73	С
ATOM		OE1 GLU B 380	49.450 19.015 65.098 1.00 70.64	0
ATOM		OE2 GLU B 380	49.588 18.269 67.182 1.00 73.27	О
ATOM		N CYSB381	47.067 23.599 66.056 1.00 45.88	N
		CA CYS B 381	47.624 24.810 66.658 1.00 44.73	С
		C CYS B 381	46.566 25.784 67.130 1.00 42.92	C
ATOM		O CYS B 381	46.792 26.395 68.178 1.00 37.98	О
ATOM		CB CYS B 381	48.572 25.454 65.635 1.00 52.09	С
ATOM		SG CYS B 381	50.273 25.860 66.085 1.00 62.86	S
ATOM		N ALA B 382	45.379 25.940 66.551 1.00 40.58	N
ATOM		CA ALAB 382	44.429 26.942 66.967 1.00 38.93	С
ATOM	2401	C ALA B 382	43.279 26.563 67.872 1.00 38.58	С
ATOM	2402		42.620 27.427 68.424 1.00 37.32	0
ATOM		CB ALA B 382	43.707 27.386 65.671 1.00 38.68	С
ATOM	2404		43.028 25.289 68.081 1.00 38.92	N
ATOM		CA TRP B 383	41.892 24.847 68.875 1.00 36.09	С
ATOM	2406		41.683 25.516 70.178 1.00 35.26	С
ATOM	2407		40.574 26.008 70.530 1.00 33.42	0
		CB TRP B 383	41.904 23.306 68.816 1.00 35.35	C.
		CG TRP B 383	42.837 22.774 69.826 1.00 33.79	C
		CD1 TRP B 383	44.153 22.436 69.663 1.00 34.99	C
		CD2 TRP B 383	42.517 22.560 71.200 1.00 32.33	C
		NE1 TRP B 383	44.662 22.021 70.857 1.00 30.51	N
		CE2 TRP B 383	43.696 22.081 71.823 1.00 29.75	C
		CE3 TRP B 383	41.355 22.750 71.944 1.00 30.48	C
		CZ2 TRP B 383	43.751 21.776 73.173 1.00 27.07	C
		CZ3 TRP B 383	41.383 22.455 73.268 1.00 31.00	C
		CH2 TRP B 383	42.591 21.963 73.857 1.00 33.85	C
		N LEUB 384	42.744 25.635 70.972 1.00 33.40	N
		CA LEUB 384	42.585 26.325 72.255 1.00 30.50	C
		C LEUB 384	42.335 27.795 72.058 1.00 31.57	C
		O LEUB 384	41.532 28.347 72.806 1.00 35.39	0
		CB LEUB 384	43.720 26.041 73.207 1.00 26.71	C
ATOM	2423	CG LEUB 384	43.548 26.567 74.605 1.00 30.98	С

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ΔΤΟΜ	2424	CDLIFTIR 384	42.142 26.159 75.119 1.00 28.22	С
			44.636 26.068 75.544 1.00 30.47	
		N GLUB 385		N
			42.672 29.904 70.872 1.00 31.19	
		C GLU B 385		
ATOM	2420	O GLUB 385	40.514 31.029 70.802 1.00 37.28	
			43.519 30.540 69.811 1.00 33.75	
ATOM	2431	CG GLUB 385	45.019 30.277 69.811 1.00 38.27	Č
			45.821 31.092 68.845 1.00 37.52	Č
ATOM	2432	OFIGUR 385	45.581 32.266 68.657 1.00 39.60	Ö
ATOM	2433	OE2 GLUB 385	46.769 30.620 68.199 1.00 44.18	Ö
			40.737 29.029 69.767 1.00 32.56	N
			39.318 29.081 69.346 1.00 32.62	C
			38.361 28.909 70.500 1.00 30.09	c
			37.359 29.606 70.692 1.00 25.95	Ö
			39.100 28.108 68.191 1.00 33.30	
			39.894 28.679 66.969 1.00 34.06	
ATOM	2441	CG2 ILE B 386	37.643 28.079 60.509 1.00 54.60	Č
ATOM	2441	CD1 II E B 386	37.643 28.026 67.815 1.00 34.81 39.864 27.634 65.882 1.00 37.55	Č
ATOM	2443	N IFILE 387	38.667 27.956 71.384 1.00 27.87	
			37.825 27.773 72.542 1.00 26.27	
			37.817 29.048 73.365 1.00 29.90	
ATOM	2446	O 1FILB 387	36.749 29.493 73.824 1.00 27.72	Ö
			38.375 26.590 73.322 1.00 23.50	
			37.930 25.215 72.829 1.00 26.32	
			38.303 24.168 73.896 1.00 21.89	
ATOM	2450	CD2 LEU B 387	36.426 25.150 72.471 1.00 21.80	Č
ATOM	2451	N MET B 388	39.039 29.641 73.530 1.00 32.23	N
			39.121 30.826 74.393 1.00 31.87	
			38.427 32.009 73.806 1.00 31.46	C
		O MET B 388	37.570 32.663 74.412 1.00 35.84	O
		CB MET B 388	40.499 31.143 74.859 1.00 31.50	С
			41.227 30.030 75.631 1.00 32.92	С
			42.970 30.484 75.860 1.00 33.47	S
		CE MET B 388	43.587 29.273 76.951 1.00 27.60	С
		N ILE B 389	38.672 32.264 72.523 1.00 30.09	N
		CA ILE B 389	37.966 33.444 71.987 1.00 25.61	С
		C ILE B 389	36,495 33,253 72,136 1.00 28,80	С
		O ILE B 389	35.793 34.263 72.389 1.00 34.46	0
ATOM	2463	CB ILE B 389	38.481 33.851 70.625 1.00 24.14	С
			38.357 35.373 70.508 1.00 25.05	С
ATOM	2465	CG2 ILE B 389	37.936 33.063 69.481 1.00 19.98	С
		CD1 ILE B 389	38.059 35.936 69.168 1.00 28.34	С
		N GLY B 390	35.932 32.076 72.040 1.00 30.54	N
		CA GLY B 390	34.488 31.888 72.191 1.00 33.74	С
		C GLY B 390	34.072 32.112 73.639 1.00 37.29	С
		O GLY B 390	33.044 32.716 73.939 1.00 36.80	0
		N LEUB 391	34.943 31.673 74.553 1.00 37.25	N
ATOM	2472	CA LEUB 391	34.604 31.848 75.994 1.00 35.83	С

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			81/371	
ATOM	2473	C LEU B 391	34.570 33.325 76.242 1.00 34.46	С
ATOM	2474	O LEU B 391	33.700 33.918 76.805 1.00 33.17	Ο
ATOM	2475	CB LEU B 391	35.734 31.153 76.794 1.00 31.89	С
ATOM	2476	CG LEUB 391	35.804 31.397 78.283 1.00 31.45	С
ATOM	2477	CD1 LEU B 391	34.434 31.098 78.962 1.00 27.42	С
ATOM	2478	CD2 LEU B 391	36.881 30.540 78.949 1.00 28.7 5	С
ATOM	2479	N VAL B 392	35.639 33.979 75.742 1.00 34.72	N
ATOM		CA VAL B 392	35.682 35.420 75.958 1.00 35.50	С
ATOM	2481	C VAL B 392	34.427 36.097 75.475 1.00 34.25	С
ATOM	2482	O VAL B 392	33.873 37.022 76.024 1.00 33.10	Ο
		CB VAL B 392	36.940 36.027 75.296 1.00 36.25	С
		CG1 VAL B 392	36.823 37.540 75.354 1.00 37.18	С
		CG2 VAL B 392	38.161 35.626 76.107 1.00 35.78	С
ATOM	2486	N TRP B 393	34.037 35.771 74.253 1.00 37.03	N
ATOM	2487	CA TRP B 393	32.918 36.461 73.632 1.00 39.42	С
ATOM		C TRP B 393	31.642 36.272 74.423 1.00 40.00	С
ATOM		O TRP B 393	30.896 37.192 74.710 1.00 42.71	0
ATOM		CB TRP B 393	32.740 35.936 72.209 1.00 37.68	C
		CG TRP B 393		C
		CD1 TRP B 393	30.405 35.350 71.438 1.00 38.63	С
		CD2 TRP B 393	30.971 37.487 71.102 1.00 35.68	С
		NE1 TRP B 393	29.324 36.007 70.826 1.00 41.40	N
		CE2 TRP B 393	29.678 37.308 70.602 1.00 37.07	С
		CE3 TRP B 393	31.542 38.740 70.957 1.00 36.83	С
		CZ2 TRP B 393	28,961 38,338 70,031 1,00 36,96	С
		CZ3 TRP B 393	30.857 39.743 70.349 1.00 33.97	С
		CH2 TRP B 393	29.553 39.557 69.920 1.00 34.11	С
		N ARG B 394	31.366 35.039 74.802 1.00 39.93	N
ATOM	2501	CA ARG B 394	30.174 34.701 75.560 1.00 36.65	С
ATOM	2502	C ARG B 394	30.229 35.138 76.994 1.00 39.01	С
ATOM	2503	O ARG B 394	. 29.194 35.311 77.694 1.00 41.96	. 0
		CB ARG B 394		С
ATOM	2505	CG ARG B 394	30.122 32.235 76.172 1.00 30.97	С
ATOM	2506	CD ARG B 394		C
ATOM	2507	NE ARG B 394	30.928 29.919 76.189 1.00 28.98	N
ATOM	2508	CZ ARG B 394	31.886 29.263 75.552 1.00 30.39	С
ATOM	2509	NH1 ARG B 394	31.995 29.476 74.222 1.00 28.81	N
ATOM	2510	NH2 ARG B 394	32.703 28.414 76.192 1.00 26.10	N
ATOM	2511	N SER B 395	31.374 35.561 77.468 1.00 39.89	N
ATOM	2512	CA SER B 395	31.581 36.128 78.784 1.00 36.60	С
ATOM	2513	C SER B 395	31.396 37.621 78.802 1.00 42.53	С
		O SER B 395	31.142 38.237 79.847 1.00 46.22	0_
		CB SER B 395	33.039 35.845 79.155 1.00 31.85	C
			33,079 34.457 79.436 1.00 28.12	0
		N MET B 396	31.520 38.302 77.688 1.00 47.19	N
		CA MET B 396	31.421 39.733 77.641 1.00 51.47	C
ATOM	2519	C MET B 396	30.489 40.366 78.647 1.00 56.34	C
ATOM			30.895 41.118 79.524 1.00 60.12	0
ATOM	2521	CB MET B 396	30.902 40.139 76.254 1.00 49.14	С

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АТОМ	2522 CG MET B 396	•	С
		31.548 41.224 73.856 1.00 42.86	
ATOM	2524 CE MET B 396	30.173 40.085 73.579 1.00 50.12	
ATOM	2525 N GLUB 397	29.212 40.096 78.533 1.00 60.93	N
ATOM	2526 CA GLUB 397	28.199 40.683 79.382 1.00 65.88	C
		27.987 39.977 80.693 1.00 66.69	
ATOM	2528 O GLUB 397	26.865 39.933 81.243 1.00 69.14	Ō
		26.895 40.725 78.560 1.00 68.52	
		27.191 41.201 77.117 1.00 70.94	
		29.052 39.472 81.294 1.00 63.21	
		29.084 38.799 82.562 1.00 62.64	C
	2536 C HIS B 398		C
		31.215 38.369 83.640 1.00 64.14	
		29.047 37.286 82.440 1.00 61.15	
		27.721 36.747 82.061 1.00 63.91	
		27.211 36.810 80.779 1.00 67.22	
		26.766 36.129 82.765 1.00 65.22	
ATOM	2542 CE1 HIS B 398	26.028 36.256 80.685 1.00 65.18	С
ATOM	2543 NE2 HIS B 398	25.756 35.822 81.899 1.00 66.32	N
ATOM	2544 N PRO B 399	30.569 40.505 83.387 1.00 63.39	N
ATOM	2545 CA PRO B 399	31.751 41.084 83.999 1.00 62.77	С
ATOM	2546 C PRO B 399	32.046 40.395 85.316 1.00 62.99	С
ATOM	2547 O PROB 399	31.131 40.222 86.121 1.00 66.99	О
		30.077 42.748 83.819 1.00 65.85	
		29.632 41.547 83.014 1.00 64.17	
		33.283 40.001 85.491 1.00 60.52	
		33.805 39.350 86.646 1.00 58.08	
		33.773 37.854 86.557 1.00 59.78	
		34.357 37.126 87.369 1.00 60.70	
ATOM	2555 N LYS B 401	33.025 37.335 85.584 1.00 61.41	N
ATOM	2556 CA LYS B 401	32.870 35.896 85.450 1.00 61.48	C
		33.127 35.416 84.033 1.00 56.79	
		32.888 36.166 83.100 1.00 57.78	
		31.394 35.554 85.812 1.00 68.06	
ATOM	2561 CD I VC D 401	31.103 35.685 87.314 1.00 72.86 29.880 34.879 87.707 1.00 77.25	C
		29.705 34.764 89.220 1.00 79.35	
		29.631 33.337 89.702 1.00 80.08	
		33.544 34.179 83.889 1.00 49.79	
		33.670 33.432 82.678 1.00 42.60	
		32.478 32.509 82.437 1.00 41.15	
	2567 O LEUB 402		
		34.960 32.546 82.682 1.00 33.63	
		36.184 33.473 82.725 1.00 32.31	
		37.502 32.732 82.793 1.00 23.92	
		36.090 34.463 81.577 1.00 30.62	
		31.775 32.667 81.328 1.00 39.54	
		30.640 31.792 81.035 1.00 39.78	

ATOM		C LEU B 403		C
ATOM			30.816 30.480 78.966 1.00 39.71	0
ATOM			29.533 32.667 80.452 1.00 42.24	C
ATOM		CG LEU B 403	28.282 32.018 79.890 1.00 43.89	C
ATOM			27.362 31.660 81.021 1.00 45.14	C
ATOM		-	27.562 32.874 78.861 1.00 43.05	C
ATOM		N PHE B 404	31.718 29.626 80.832 1.00 40.77	N
ATOM	2581	CA PHE B 404	32.176 28.419 80.149 1.00 39.29	С
ATOM	2582		30.962 27.790 79.501 1.00 40.29	C
ATOM	2583			0
ATOM			32.905 27.438 81.026 1.00 37.12	C
ATOM		CG PHE B 404		C
ATOM			34.333 28.785 82.593 1.00 35.02	С
ATOM			35.395 27.576 80.848 1.00 31.59	C
ATOM			35,587 29,241 83,023 1,00 37,43	C
ATOM			36.616 28.005 81.263 1.00 30.58	C
ATOM	2590		36.740 28.838 82.341 1.00 33.26	С
ATOM	2591		29.828 27.789 80.137 1.00 41.67	N
ATOM		,	28.558 27.337 79.623 1.00 39.74	С
ATOM		C ALA B 405		C
		O ALA B 405	27.723 28.829 81.314 1.00 45.02	0
ATOM		CB ALA B 405	28.274 25.894 79.888 1.00 38.06	C
			26.272 28.127 79.754 1.00 41.38	N
		CA PRO B 406	25.134 28.819 80.323 1.00 39.78	C
ATOM		C PRO B 406	24.922 28.230 81.704 1.00 43.39	C
ATOM	2599		24.687 28.978 82.635 1.00 47.07	0
ATOM		CB PRO B 406	23.942 28.571 79.409 1.00 39.54	C
ATOM		CG PRO B 406	24.615 28.101 78.150 1.00 39.07	C
ATOM		CD PRO B 406	25.913 27.404 78.549 1.00 40.30	C
ATOM		N ASN B 407		N
ATOM			24.938 26.334 83.217 1.00 44.35	C
ATOM		C ASN B 407		C
ATOM		O ASN B 407	26.358 25.322 84.859 1.00 43.21	0
		CB ASN B 407	24.207 24.990 83.095 1.00 45.30	C
		CG ASN B 407	25.102 23.905 82.560 1.00 48.52	
		-	26.017 24.173 81.765 1.00 52.75	0
		ND2 ASN B 407	24.868 22.682 82.982 1.00 47.55 27.230 26.971 83.581 1.00 44.78	N N
		N LEUB 408	28.530 26.840 84.245 1.00 43.66	C
		CA LEUB 408		c
		C LEUB 408	29.274 28.160 84.105 1.00 46.96 30.177 28.206 83.300 1.00 47.50	Ö
		O LEUB 408	29.348 25.734 83.640 1.00 47.30	C
		CB LEUB 408	30.702 25.450 84.231 1.00 41.46	C
		CG LEUB 408		C
		CD1 LEU B 408	30.579 25.028 85.691 1.00 43.35 31.454 24.396 83.439 1.00 40.80	C
		CD2 LEU B 408		N
		N LEUB 409	28.857 29.155 84.856 1.00 49.18 29.399 30.474 84.971 1.00 51.85	C
		CA LEUB 409	30.384 30.538 86.149 1.00 54.53	C
ATOM				Ö
ATOM	2022	O LEU B 409	29.967 30.547 87.300 1.00 57.83	J

		•	
ATOM	2672 CA GLY B 415	39.053 29.370 88.813 1.00 87.32	С
ATOM	2673 C GLY B 415	40.291 29.004 89.616 1.00 87.9 9	С
ATOM	2674 O GLY B 415	41.156 28.238 89.181 1.00 86.24	О
ATOM	2675 N LYS B 416	40.364 29.509 90.842 1.00 90.55	N
ATOM	2676 CA LYS B 416	41.442 29.218 91.767 1.00 93.58	С
ATOM	2677 C LYS B 416	41.561 27.754 92.141 1.00 95.38	С
ATOM	2678 O LYS B 416	42.671 27.241 92.349 1.00 95.66	0
ATOM	2679 CB LYS B 416	41.269 30.074 93.037 1.00 93.15	С
ATOM	2684 N CYS B 417	40.489 26.977 92.152 1.00 97.58	N
ATOM	2685 CA CYS B 417	40.448 25.571 92.472 1.00100.45	С
ATOM	2686 C CYS B 417	41.276 24.692 91.543 1.00 99.99	С
ATOM	2687 O CYS B 417	41.292 23.457 91.586 1.00 99.87	0
ATOM	2688 CB CYS B 417	39.005 25.045 92.445 1.00103.57	С
ATOM	2689 SG CYS B 417	37.717 25.947 93.323 1.00109.90	S
ATOM	2690 N VAL B 418	41.992 25.273 90.607 1.00 99.92	N
ATOM	2691 CA VAL B 418	42.857 24.622 89.651 1.00 99.16	С
ATOM	2692 C VAL B 418	44.197 25.380 89.670 1.00 98.34	С
ATOM	2693 O VAL B 418	44.186 26.600 89.508 1.00 97.73	0
ATOM	2694 CB VAL B 418	42.303 24.667 88.218 1.00 99.72	С
ATOM	2695 CG1 VAL B 418	43.007 23.621 87.358 1.00 97.84	С
ATOM	2696 CG2 VAL B 418	40.795 24.517 88.146 1.00 98.53	С
ATOM	2697 N GLUB 419	45.278 24.673 89.873 1.00 98.42	N
ATOM	2698 CA GLUB 419	46.605 25.274 89.952 1.00 98.68	C
ATOM	2699 C GLU B 419	47.104 25.893 88.661 1.00 97.48	С
ATOM	2700 O GLUB 419	47.289 25.222 87.639 1.00 98.90	Ο
ATOM	2701 CB GLU B 419	47.598 24.230 90.490 1.00 99.66	С
ATOM	2706 N GLY B 420	47.362 27.207 88.696 1.00 94.17	N
ATOM	2707 CA GLY B 420	47.816 27.918 87.511 1.00 91.36	С
ATOM	2708 C GLY B 420	46.684 28.553 86.708 1.00 88.54	С
ATOM	2709 O GLY B 420	46.918 29.464 85.895 1.00 88.73	O
ATOM	2710 N MET B 421	45.435 28.140 86.958 1.00 83.23	N
	2711 CA MET B 421	44.336 28.679 86.203 1.00 80.10	С
ATOM	2712 C MET B 421	44.023 30.138 86.465 1.00 76.64	C
	2713 O MET B 421	43.546 30.845 85.548 1.00 77.79	0
	2714 CB MET B 421	43.107 27.781 86.353 1.00 80.33	C
	2715 CG MET B 421	42.062 28.036 85.275 1.00 79.26	C
	2716 SD MET B 421	40.735 26.848 85.309 1.00 79.88	S
	2717 CE MET B 421	41.509 25.424 84.511 1.00 78.20	C
	2718 N VAL B 422	44.329 30.649 87.633 1.00 70.06	N
	2719 CA VAL B 422	44.014 32.028 87.971 1.00 66.93	C
	2720 C VAL B 422	44.617 33.051 87.034 1.00 62.98	C
	2721 O VAL B 422	43.970 33.990 86.582 1.00 59.44	0
	2722 CB VAL B 422	44.481 32.384 89.405 1.00 67.44	C
	2723 CG1 VAL B 422	43.588 33.465 89.994 1.00 66.70	C
	2724 CG2 VAL B 422	44.478 31.117 90.259 1.00 69.52	C
	2725 N GLUB 423	45.911 32.877 86.738 1.00 62.98	N
ATOM		46.561 33.863 85.854 1.00 60.72	С
	2727 C GLUB 423	45.900 33.831 84.486 1.00 56.94	C
ATOM	2728 O GLUB 423	45.496 34.892 83.976 1.00 58.86	О

			48.059 33.742 85.792 1.00 59.28	
			45.629 32.636 83.964 1.00 50.05	N
			44.981 32.635 82.652 1.00 48.51	С
		C ILE B 424		С
		O ILE B 424		0
			45.041 31.288 81.951 1.00 44.17	С
			46.526 30.904 81.777 1.00 41.42	С
			44.420 31.454 80.588 1.00 40.80	С
		CD1 ILE B 424		С
ATOM	2742	N PHE B 425	42.905 32.732 83.813 1.00 49.07	N
ATOM	2743	CA PHE B 425	41.562 33.166 84.131 1.00 49.17	С
ATOM	2744	C PHE B 425	41.450 34.686 84.190 1.00 49.03	С
ATOM	2745	O PHE B 425	40.517 35.354 83.723 1.00 46.73	0
ATOM	2746	CB PHE B 425	41.241 32.595 85.529 1.00 51.92	С
ATOM	2747	CG PHE B 425	39.762 32.392 85.709 1.00 51.58	С
ATOM	2748	CD1 PHE B 425	38.960 33.504 85.864 1.00 53.18	С
ATOM	2749	CD2 PHE B 425	39.212 31.134 85.713 1.00 50.30	С
ATOM	2750	CE1 PHE B 425	37.593 33.370 86.021 1.00 54.70	С
			37.858 30.966 85.875 1.00 51.75	С
ATOM	2752	CZ PHE B 425	37.049 32.078 86.029 1.00 54.42	С
ATOM	2753	N ASP B 426	42.475 35.304 84.790 1.00 48.98	N
ATOM	2754	CA ASP B 426	42.505 36.760 84.888 1.00 48.73	С
		C ASP B 426		С
ATOM	2756	O ASP B 426	42.027 38.412 83.218 1.00 46.68	0
ATOM	2757	CB ASP B 426	43.708 37.168 85.736 1.00 52.22	С
ATOM	2758	CG ASP B 426	43.343 37.213 87.204 1.00 52.65	С
ATOM	2759	OD1 ASP B 426	42.139 37.339 87.499 1.00 54.85	Ο
ATOM	2760	OD2 ASP B 426	44.300 37.109 87.971 1.00 55.57	0
ATOM	2761	N MET B 427	43.495 36.795 82.730 1.00 44.72	N
ATOM	2762	CA MET B 427	43.797 37.174 81.364 1.00 41.75	С
ATOM	2763	C MET B 427	42.544 37.067 80.504 1.00 39.43	С
ATOM	2764	O MET B 427	42.155 37.984 79.789 1.00 39.81	Ο
ATOM	2765	CB MET B 427	44.907 36.188 80.884 1.00 44.36	С
ATOM	2766	CG MET B 427	46.294 36.729 81.084 1.00 48.85	С
ATOM	2767	SD MET B 427	47.678 35.780 80.492 1.00 55.91	S
ATOM	2768	CE MET B 427	47.419 34.154 81.133 1.00 52.49	С
ATOM	2769	N LEUB 428	41.814 35.942 80.690 1.00 35.14	N
ATOM	2770	CA LEUB 428	40.580 35.698 79.969 1.00 34.18	С
ATOM	2771	C LEU B 428	39.597 36.778 80.362 1.00 34.40	С
ATOM	2772	O LEU B 428	39.044 37.473 79.523 1.00 35.33	0
ATOM	2773	CB LEUB 428	39.989 34.299 80.162 1.00 30.49	С
ATOM	2774	CG LEUB 428	40.876 33.217 79.482 1.00 28.71	С
ATOM	2775	CD1 LEU B 428	40.714 31.829 79.995 1.00 26.98	С
ATOM	2776	CD2 LEU B 428	40.656 33.261 78.002 1.00 29.20	С
		N LEU B 429	39.562 37.071 81.667 1.00 37.03	N
		CA LEUB 429	38.678 38.138 82.109 1.00 35.92	С
		C LEUB 429	39.005 39.465 81.457 1.00 35.69	С
		O LEU B 429	38.047 40.111 80.996 1.00 33.54	0
		CB LEU B 429	38.703 38.277 83.621 1.00 32.15	С

ATOM 2782 CG LEU B 429 37,830 37.222 84.321 1.00 33.08 38.082 37.290 85.814 1.00 27.55 ATOM 2783 CD1 LEU B 429 ATOM 2784 CD2 LEU B 429 36,362 37,329 83,909 1,00 29,01 C ATOM 2785 N ALA B 430 40.296 39.813 81.393 1.00 32.95 ATOM 2786 CA ALA B 430 40.634 41.126 80.826 1.00 36.84 C 40.338 41.228 79.335 1.00 38.44 C ATOM 2787 C ALA B 430 ATOM 2788 O ALA B 430 39.968 42.264 78.761 1.00 36.45 0 ATOM 2789 CB ALA B 430 42.102 41.541 81.010 1.00 34.40 C ATOM 2790 N THR B 431 40.580 40.079 78.661 1.00 37.54 N ATOM 2791 CA THR B 431 40.159 40.081 77.252 1.00 36.70 C ATOM 2792 C THR B 431 38.676 40.337 77.081 1.00 37.98 ATOM 2793 O THR B 431 38.287 41.142 76.201 1.00 35.69 0 ATOM 2794 CB THR B 431 40.645 38.754 76.682 1.00 35.10 C 42.064 38.624 77.003 1.00 38.56 ATOM 2795 OG1 THR B 431 ATOM 2796 CG2 THR B 431 40,434 38.713 75.188 1.00 31.41 C ATOM 2797 N SER B 432 37,747 39.703 77.877 1.00 39.84 ATOM 2798 CA SER B 432 36.344 39.976 77.574 1.00 45.36 C 36,025 41.411 77.977 1.00 43.30 ATOM 2799 C SER B 432 C 35.274 42.080 77.282 1.00 42.62 ATOM 2800 O SER B 432 0 ATOM 2801 CB SER B 432 35.225 39.117 78.140 1.00 45.94 C ATOM 2802 OG SER B 432 35.659 38.558 79.329 1.00 49.61 ATOM 2803 N SER B 433 36.744 41.837 78.999 1.00 43.13 N ATOM 2804 CA SER B 433 36.535 43.234 79.330 1.00 46.73 C ATOM 2805 C SER B 433 36.855 44.133 78.146 1.00 46.01 C ATOM 2806 O SER B 433 36.086 45.008 77.734 1.00 49.24 O ATOM 2807 CB SER B 433 37.281 43.646 80.573 1.00 49.56 C ATOM 2808 OG SER B 433 37.206 45.117 80.541 1.00 58.60 0 ATOM 2809 N ARG B 434 37.992 43.977 77.531 1.00 45.21 N ATOM 2810 CA ARG B 434 38.409 44.760 76.382 1.00 44.15 C ATOM 2811 C ARG B 434 37.442 44.548 75.237 1.00 45.33 ATOM 2812 O ARG B 434 37.074 45.482 74.494 1.00 45.12 0 ATOM 2813 CB ARG B 434 39.835 44.290 76.082 1.00 46.77 ATOM 2814 CG ARG B 434 40.513 45.050 74.967 1.00 55.03 ATOM 2815 CD ARG B 434 40.600 46.516 75.253 1.00 61.34 ATOM 2816 NE ARG B 434 40.638 47.463 74.192 1.00 66.92 N ATOM 2817 CZ ARG B 434 41.455 47.618 73.169 1.00 70.57 ATOM 2818 NH1 ARG B 434 42.477 46.762 73.004 1.00 73.65 N 41,260 48,625 72,314 1.00 69,23 ATOM 2819 NH2 ARG B 434 N ATOM 2820 N PHE B 435 36.897 43.321 75.074 1.00 44.07 N ATOM 2821 CA PHE B 435 35.874 43.158 74.043 1.00 44.36 C ATOM 2822 C PHE B 435 34.672 44.042 74.362 1.00 42.27 C ATOM 2823 O PHE B 435 34.122 44.594 73.437 1.00 40.63 0 ATOM 2824 CB PHE B 435 35.460 41.727 73.743 1.00 44.13 C ATOM 2825 CG PHE B 435 36.410 40.882 72.948 1.00 46.42 ATOM 2826 CD1 PHE B 435 37.432 41.396 72.187 1.00 47.77 C ATOM 2827 CD2 PHE B 435 36.310 39.505 72.955 1.00 48.65 ATOM 2828 CE1 PHE B 435 38.314 40.645 71.467 1.00 46.44 ATOM 2829 CE2 PHE B 435 37.178 38.706 72.249 1.00 50.86 C ATOM 2830 CZ PHE B 435 38.196 39.278 71.493 1.00 49.02

ATOM	2831	N ARG B 436	34.265 44.140 75.618 1.00 45.66	N
			33.117 44.927 76.027 1.00 49.37	С
ATOM		C ARG B 436		C
ATOM	2834	O ARG B 436		O
ATOM		CB ARG B 436		С
ATOM		CG ARG B 436		C
ATOM		CD ARG B 436		Č
ATOM		NE ARGB 436		N
ATOM		CZ ARG B 436		C
ATOM		NHI ARG B 436		N
ATOM	2841	NH2 ARG B 436	33.260 42.010 80.867 1.00 60.90	N
ATOM		N MET B 437	·	N
ATOM		CA MET B 437		Ċ
ATOM		C MET B 437	34.892 48.497 74.611 1.00 54.67	c
ATOM	2845	O MET B 437	34.292 49.542 74.301 1.00 56.44	Ö
ATOM		CB MET B 437		Č
-			36.614 49.111 77.788 1.00 74.21	Č
		SD MET B 437		S
ATOM		CE MET B 437		č
ATOM		N MET B 438		N
ATOM	2851	CA MET B 438		C
ATOM		C MET B 438	33.977 47.842 71.604 1.00 46.47	c
ATOM		O MET B 438	33.850 47.985 70.374 1.00 46.26	Ö
ATOM		CB MET B 438	36.371 47.632 71.348 1.00 46.13	C
ATOM			37.616 47.220 72.115 1.00 44.79	Č
			38.883 46.590 71.100 1.00 46.76	S
ATOM			38.508 47.061 69.426 1.00 42.55	Č
ATOM		N ASN B 439		N
ATOM			31.769 46.909 71.719 1.00 47.08	С
ATOM	2860			C
ATOM	2861	O ASN B 439		Ō
ATOM			30.894 48.043 71.160 1.00 54.41	С
ATOM			30.681 49.113 72.228 1.00 62.82	С
		OD1 ASN B 439	30.400 48.772 73.391 1.00 68.45	0
		ND2 ASN B 439	30.853 50.398 71.948 1.00 63.44	N
		N LEUB 440	32.836 44.915 70.767 1.00 40.15	N
		CA LEUB 440	33.036 43.990 69.681 1.00 38.02	С
		C LEUB 440	31.700 43.440 69.201 1.00 39.56	С
		O LEUB 440	30.812 43.082 69.978 1.00 39.57	Ο
		CB LEUB 440	33.945 42.860 70.083 1.00 39.03	С
		CG LEUB 440	34.095 41.816 68.957 1.00 38.64	С
		CD1 LEU B 440	34.882 42.503 67.863 1.00 40.77	С
		CD2 LEU B 440	34.781 40.613 69.567 1.00 40.57	С
		N GLN B 441	31.563 43.417 67.890 1.00 40.69	N
		CA GLN B 441	30.317 43.001 67.272 1.00 40.46	С
		C GLN B 441	30.476 41.572 66.796 1.00 41.61	С
		O GLN B 441	31.573 41.135 66.435 1.00 42.47	Ο
		CB GLN B 441		С
		CG GLN B 441	29.793 45.380 66.436 1.00 48.63	С
	-			

			89/371	
ATOM	2880	CD GLN B 441	28.646 45.620 67.426 1.00 53.79	С
ATOM	2881	OE1 GLN B 441	27.473 45.380 67.078 1.00 57.83	0
ATOM	2882	NE2 GLN B 441	28.952 46.095 68.623 1.00 50.24	N
ATOM	2883	N GLY B 442	29.358 40.858 66.803 1.00 39.15	N
ATOM	2884	CA GLY B 442	29.364 39.473 66.404 1.00 38.36	С
ATOM	2885	C GLY B 442	29.980 39.287 65.030 1.00 38.59	С
ATOM	2886	O GLY B 442	30.700 38.317 64.869 1.00 36.85	Ō
ATOM	2887	N GLU B 443	29.673 40.200 64.107 1.00 39.06	N
ATOM	2888	CA GLUB 443	30.225 40.130 62.778 1.00 40.77	C
		C GLU B 443	31.747 40.195 62.764 1.00 38.88	C
ATOM		O GLUB 443	32.341 39.502 61.958 1.00 40.31	ŏ
ATOM		CB GLUB 443	29.725 41.274 61.885 1.00 43.92	Č
ATOM		CG GLUB 443	28.280 40.999 61.489 1.00 49.93	Č
ATOM		CD GLUB 443	27.289 41.423 62.556 1.00 52.01	Č
ATOM		OE1 GLU B 443	27.607 42.080 63.559 1.00 52.95	Ö
ATOM		OE2 GLU B 443	26.103 41.072 62.367 1.00 56.50	ŏ
		N GLU B 444	32.304 41.015 63.624 1.00 36.15	N
		CA GLUB 444	33.718 41.205 63.814 1.00 34.58	Ċ
ATOM		C GLU B 444	34.304 39.991 64.512 1.00 33.55	Č
ATOM		O GLU B 444	35.328 39.436 64.169 1.00 37.22	ŏ
ATOM		CB GLUB 444	33.958 42.439 64.667 1.00 34.86	Č
ATOM		CG GLU B 444	33.459 43.740 64.094 1.00 31.42	Č
ATOM		CD GLU B 444	33.675 44.906 65.062 1.00 34.07	Č
ATOM		OE1 GLU B 444	33.134 44.858 66.203 1.00 30.06	Ŏ
ATOM		OE2 GLU B 444	34.371 45.875 64.646 1.00 31.32	ŏ
ATOM		N PHE B 445	33.608 39.484 65.490 1.00 36.24	N
ATOM		CA PHE B 445	34.003 38.295 66.254 1.00 35.58	Ĉ
ATOM		C PHE B 445	34.308 37.128 65.357 1.00 35.27	c
ATOM	2908	O PHE B 445	35.313 36.412 65.412 1.00 40.19	ŏ
ATOM		CB PHE B 445	32.830 37.907 67.202 1.00 29.13	C
ATOM		CG PHE B 445	32.976 36.563 67.791 1.00 25.96	č
ATOM		CD1 PHE B 445	34.034 36.211 68.566 1.00 25.60	C
		CD2 PHE B 445	32.009 35.585 67.537 1.00 28.36	Č
		CE1 PHE B 445		C
		CE2 PHE B 445	32.014 34.314 68.054 1.00 26.68	Č
		CZ PHE B 445	33.127 33.951 68.828 1.00 28.70	Č
		N VAL B 446	33.340 36.823 64.553 1.00 34.10	N
		CA VALB 446	33.325 35.647 63.645 1.00 34.65	C
		C VAL B 446	34.441 35.755 62.659 1.00 35.98	C
		O VAL B 446	35.089 34.817 62.161 1.00 35.51	Ö
		CB VALB 446	31.855 35.683 63.194 1.00 34.90	Č
		CG1 VAL B 446	31.527 35.886 61.769 1.00 32.60	Č
ATOM		CG2 VAL B 446	31.123 34.554 63.911 1.00 32.13	Č
ATOM		N CYS B 447	34.751 37.011 62.335 1.00 36.12	N
		CA CYS B 447	35.830 37.341 61.416 1.00 36.00	Ĉ
		C CYS B 447	37.163 37.010 62.071 1.00 37.62	Č
		O CYS B 447	38.056 36.366 61.498 1.00 37.88	ŏ
		CB CYS B 447	35.638 38.810 61.119 1.00 35.26	C
		SG CYS B 447	34.873 39.112 59.520 1.00 36.98	Š
AT OW	2720	ודד ענגט טכו	JT.073 J7.112 J7.J20 1.00 J0.70	S

ATOM 2930 CA LEUB 448 ATOM 2931 C LEUB 448 ATOM 2932 O LEUB 448 39.852 35.258 64.471 1.00 33.33 0 ATOM 2933 CB LEU B 448 38.420 37.971 65.400 1.00 35.13 ATOM 2934 CG LEUB 448 38.540 39.490 65.512 1.00 32.37 ATOM 2935 CD1 LEU B 448 38.938 39.710 66.999 1.00 33.43 39,657 40,004 64,637 1.00 33.31 ATOM 2936 CD2 LEU B 448 ATOM 2937 N LYS B 449 37.641 34.906 64.606 1.00 31.66 N 37.843 33.470 64.808 1.00 30.93 C ATOM 2938 CA LYS B 449 ATOM 2939 C LYS B 449 38.462 32.865 63.553 1.00 29.14 39.333 32.064 63.717 1.00 32.42 ATOM 2940 O LYS B 449 0 ATOM 2941 CB LYS B 449 36.623 32.626 65.068 1.00 31.04 C ATOM 2942 CG LYS B 449 36.177 32.488 66.496 1.00 36.23 35.310 31.208 66.665 1.00 34.18 ATOM 2943 CD LYS B 449 ATOM 2944 CE LYS B 449 33.890 31.672 66.346 1.00 33.96 ·C ATOM 2945 NZ LYS B 449 32.896 30.611 66.205 1.00 32.13 N ATOM 2946 N SER B 450 37.937,33.118 62.384 1.00 29.89 N ATOM 2947 CA SER B 450 38.485 32.554 61.162 1.00 33.15 C ATOM 2948 C SER B 450 39.948 32.941 60.947 1.00 33.99 C ATOM 2949 O SER B 450 40.741 32.059 60.569 1.00 36.13 0 ATOM 2950 CB SER B 450 37.677 33.112 59.971 1.00 35.66 C ATOM 2951 OG SER B 450 36.448 32.390 59.964 1.00 42.36 0 ATOM 2952 N ILE B 451 N 40,291 34,212 61,179 1,00 28,73 41.689 34.636 61.077 1.00 28.97 C ATOM 2953 CA ILE B 451 42.542 33.780 62.024 1.00 30.60 ATOM 2954 C ILE B 451 43.622 33.306 61.687 1.00 34.48 0 ATOM 2955 O ILE B 451 C ATOM 2956 CB ILE B 451 41.877 36.109 61.474 1.00 26.02 41.408 37.037 60.331 1.00 23.22 ATOM 2957 CG1 ILE B 451 ATOM 2958 CG2 ILE B 451 43.361 36.401 61.672 1.00 29.64 C 41.256 38.461 60.801 1.00 18.98 ATOM 2959 CD1 ILE B 451 ATOM 2960 N ILE B 452 42.099 33.533 63.249 1.00 30.12 N 42.843 32.711 64.175 1.00 29.93 C ATOM 2961 CA ILE B 452 ATOM 2962 C ILE B 452 43.056 31.337 63.559 1.00 31.42 ATOM 2963 O ILE B 452 44.195 30.815 63.582 1.00 34.08 0 ATOM 2964 CB ILE B 452 42.144 32.606 65.550 1.00 28.86 42.345 33.913 66.330 1.00 26.71 ATOM 2965 CG1 ILE B 452 ATOM 2966 CG2 ILE B 452 42.556 31.429 66.392 1.00 22.07 C ATOM 2967 CD1 ILE B 452 41.556 33.907 67.645 1.00 25.52 C ATOM 2968 N LEUB 453 42.019 30.719 63.057 1.00 30.00 N ATOM 2969 CA LEUB 453 42.178 29.363 62.504 1.00 33.56 C ATOM 2970 C LEU B 453 43,230 29,315 61,378 1,00 34,89 C ATOM 2971 O LEUB 453 44.116 28.440 61.327 1.00 31.76 0 ATOM 2972 CB LEUB 453 40.849 28.894 61.906 1.00 31.42 ATOM 2973 CG LEU B 453 40.852 27.667 61.019 1.00 28.92 ATOM 2974 CD1 LEU B 453 41.063 26.366 61.798 1.00 24.08 C ATOM 2975 CD2 LEU B 453 39.503 27.591 60.278 1.00 30.58 C ATOM 2976 N LEUB 454 43.077 30.262 60.454 1.00 34.10 N ATOM 2977 CA LEUB 454 43.928 30.393 59.312 1.00 35.40

ATOM 3027 N TYR B 459 52.686 28.951 59.520 1.00101.08 N ATOM 3028 CA TYR B 459 54.118 28.829 59.478 1.00105.58 C ATOM 3029 C TYR B 459 54.628 27.383 59.505 1.00106.66 C ATOM 3030 O TYR B 459 55.476 27.053 60.360 1.00106.92 0 54.759 29.538 60.691 1.00108.78 ATOM 3031 CB TYR B 459 54.932 31.015 60.441 1.00112.75 ATOM 3032 CG TYR B 459 54.140 31.670 59.507 1.00114.02 C ATOM 3033 CD1 TYR B 459 C ATOM 3034 CD2 TYR B 459 55.888 31.764 61.118 1.00113.67 ATOM 3035 CE1 TYR B 459 54.269 33.009 59.243 1.00114.56 56.030 33.115 60.860 1.00114.48 C ATOM 3036 CE2 TYR B 459 ATOM 3037 CZ TYR B 459 55.220 33.728 59.937 1.00114.74 C ATOM 3038 OH TYR B 459 55.309 35.074 59.662 1.00115.64 O ATOM 3039 N LEUB 469 53.455 26.042 47.196 1.00114.47 N ATOM 3040 CA LEUB 469 53.703 27.415 47.649 1.00113.63 C ATOM 3041 C LEUB 469 52.595 28.339 47.164 1.00111.18 С ATOM 3042 O LEUB 469 52.452 29.481 47.572 1.00110.61 0 55.056 27.927 47.145 1.00114.74 C ATOM 3043 CB LEU B 469 51.735, 27.749 46.323 1.00108.99 ATOM 3047 N GLUB 470 ATOM 3048 CA GLUB 470 50.552 28.514 45.891 1.00107.74 C 49.492 28.303 46.983 1.00106.21 ATOM 3049 C GLUB 470 C ATOM 3050 O GLUB 470 48.424 28.886 46.982 1.00106.32 0 ATOM 3051 CB GLUB 470 50.083 28.142 44.510 1.00107.28 C ATOM 3056 N GLUB 471 49.832 27.431 47.915 1.00103.94 N 49.046 27.060 49.063 1.00102.02 C ATOM 3057 CA GLU B 471 49.190 28.135 50.131 1.00 99.15 ATOM 3058 C GLU B 471 ATOM 3059 O GLU B 471 48.228 28.784 50.542 1.00100.18 0 ATOM 3060 CB GLUB 471 49.505 25.692 49.591 1.00102.87 C ATOM 3065 N LYS B 472 50.438 28,412 50.518 1.00 95.05 N 50.694 29.474 51.488 1.00 90.18 C ATOM 3066 CA LYS B 472 ATOM 3067 C LYS B 472 49.906 30.708 51.018 1.00 85.61 C ATOM 3068 O LYS B 472 49.154 31.313 51.764 1.00 85.79 0 C 52.164 29.863 51.584 1.00 90.78 ATOM 3069 CB LYS B 472 ATOM 3074 N ASP B 473 50.106 30.995 49.743 1.00 79.96 N ATOM 3075 CA ASP B 473 49.463 32.091 49.096 1.00 76.18 C ATOM 3076 C ASP B 473 47.971 32.104 49.117 1.00 70.30 C ATOM 3077 O ASP B 473 47.343 33.158 49.225 1.00 68.00 0 ATOM 3078 CB ASP B 473 50.058 32.230 47.670 1.00 79.82 C ATOM 3079 CG ASP B 473 50.812 33.579 47.744 1.00 85.00 51.707 33.695 48.625 1.00 87.11 ATOM 3080 OD1 ASP B 473 О ATOM 3081 OD2 ASP B 473 50.338 34.479 47.015 1.00 86.01 0 47.315 30.960 49.042 1.00 67.17 N ATOM 3082 N HIS B 474 ATOM 3083 CA HIS B 474 45.859 30.919 49.049 1.00 64.04 C C ATOM 3084 C HISB 474 45.313 31.500 50.359 1.00 59.13 44.512 32.421 50.406 1.00 54.26 ATOM 3085 O HIS B 474 0 ATOM 3086 CB HIS B 474 45.373 29.472 48.872 1.00 65.44 C 43.869 29.373 48.910 1.00 66.08 C ATOM 3087 CG HIS B 474 N ATOM 3088 ND1 HIS B 474 43.042 30.096 48.057 1.00 64.73 C ATOM 3089 CD2 HIS B 474 43.085 28.640 49.749 1.00 63.86 41.788 29.791 48.371 1.00 65.57 C ATOM 3090 CE1 HIS B 474

			41.798 28.914 49.383 1.00 65.82	N
ATOM		N ILEB 475	45.796 30.880 51.428 1.00 54.85	N
ATOM		CA ILE B 475		C
ATOM		C ILE B 475	45.684 32.719 52.997 1.00 52.67	C
ATOM		O ILE B 475	44.795 33.382 53.573 1.00 52.33	O C
ATOM		CB ILE B 475	46.369 30.407 53.743 1.00 53.77	C
			45.613 29.092 54.003 1.00 55.72	C
ATOM			46.702 31.124 55.023 1.00 50.98	C
ATOM		CD1 ILE B 475	45.981 28.459 55.332 1.00 57.41 46.807 33.259 52.541 1.00 51.23	N
ATOM		N HIS B 476		C
ATOM		CA HIS B 476		C
		C HIS B 476	46.068 35.544 51.960 1.00 57.23	Ö
		O HIS B 476	45.771 36.671 52.356 1.00 59.56	·C
		CB HIS B 476		C
			49.496 34.811 53.217 1.00 73.21	_
		ND1 HIS B 476	50.291 33.686 53.347 1.00 76.61	N C
		CD2 HIS B 476	49.789 35.602 54.290 1.00 75.57	C
		CE1 HIS B 476		N
ATOM		NE2 HIS B 476		N
		N ARG B 477	45.511 35.068 50.862 1.00 55.52	C
		CA ARG B 477	44.499 35.781 50.123 1.00 55.00	C
		C ARG B 477	43.171 35.727 50.840 1.00 51.68	0
		O ARG B 477		C
		CB ARG B 477		C
		CG ARG B 477		C
		CD ARGB 477		N
		NE ARG B 477	42.939 34.574 51.496 1.00 48.24	N
		N VAL B 478		C
		CA VAL B 478	41.733 35.408 53.425 1.00 43.33	c
		C VAL B 478		Ö
ATOM		• •	• .	C
		CB VAL B 478 CG1 VAL B 478		C
ATOM				C
		CG2 VAL B 478 N LEU B 479	42.928 35.425 54.060 1.00 42.57	N
		CA LEU B 479		Ċ
		C LEU B 479	43.018 37.825 54.643 1.00 38.95	c
		O LEUB 479	42.407 38.618 55.374 1.00 44.89	ŏ
		CB LEU B 479	44.598 36.247 55.697 1.00 38.43	Č
		CG LEU B 479		č
		CD1 LEU B 479		Č
		CD2 LEU B 479		Č
		N ASP B 480	43.481 38.218 53.498 1.00 37.41	N
		CA ASP B 480	43.276 39.561 52.966 1.00 39.12	Ċ
		CA ASP B 480	41.776 39.859 52.822 1.00 39.72	Č
		O ASP B 480	41.244 40.935 53.171 1.00 37.31	ŏ
		CB ASP B 480		C
		CG ASP B 480		Č
		OD1 ASP B 480		Ō
AT OIVI	J 144	ODIAGID 400	10.017 70.171 32.037 1.00 15.00	•

ATOM	3143	OD2 ASP B 480	45.934 40.346 50.526 1.00 50.28	0
			41.060 38.846 52.311 1.00 37.19	N
ATOM	3145	CA LYS B 481	39.626 39.005 52.153 1.00 39.36	С
ATOM	3146	C LYS B 481	38.942 39.231 53.490 1.00 37.52	С
ATOM	3147	O LYS B 481	38.052 40.083 53.640 1.00 33.55	Ο
ATOM	3148	CB LYS B 481	39.076 37.807 51.405 1.00 44.24	С
			37.767 38.132 50.733 1.00 51.43	С
ATOM	3150	CD LYS B 481	37.705 37.779 49.253 1.00 54.23	С
ATOM	3151	CE LYS B 481	36.592 38.657 48.653 1.00 55.57	С
ATOM	3152	NZ LYS B 481	37.061 39.411 47.470 1.00 60.01	N
ATOM	3153	N ILE B 482	39.455 38.536 54.537 1.00 35.79	N
ATOM	3154	CA ILE B 482	38.872 38.765 55.867 1.00 33.69	С
ATOM	3155	C ILE B 482	39.141 40.146 56.389 1.00 34.23	С
ATOM	3156	O ILE B 482	38.239 40.803 56.970 1.00 35.10	Ο
ATOM	3157	CB ILE B 482	39.092 37.644 56.819 1.00 31.16	С
ATOM	3158	CG1 ILE B 482	38.922 36.299 56.067 1.00 24.05	С
ATOM	3159	CG2 ILE B 482	38.101 37.675 57.989 1.00 31.64	С
ATOM	3160	CD1 ILE B 482	38.933 35.211 57.089 1.00 25.98	С
ATOM	3161	N THR B 483	40.332 40.657 56.099 1.00 33.25	N
ATOM	3162	CA THR B 483	40.643 42.033 56.499 1.00 33.50	С
ATOM	3163	C THR B 483	39.644 42.958 55.811 1.00 35.50	С
ATOM	3164	O THR B 483	39.015 43.787 56.417 1.00 36.34	Ο
ATOM	3165	CB THR B 483	42.066 42.428 56.055 1.00 32.03	С
			43.012 41.542 56.714 1.00 31.73	O
			42.368 43.871 56.435 1.00 23.76	С
		N ASP B 484		N
ATOM	3169	CA ASP B 484	38.526 43.498 53.678 1.00 39.14	С
		C ASP B 484		С
		O ASP B 484		0_
			38.415 42.904 52.293 1.00 42.39	C
			39.624 43.139 51.453 1.00 45.80	·C
			40.287 44.189 51.613 1.00 51.95	0
ATOM		OD2 ASP B 484	39.958 42.283 50.636 1.00 48.98	0
		N THR B 485	36.702 42.236 54.635 1.00 36.36	N
		CA THR B 485		C
		C THR B 485	35.396 42.874 56.589 1.00 39.62	C
		O THR B 485	34.469 43.641 56.847 1.00 42.09	0
		CB THR B 485	35.092 40.639 55.602 1.00 35.78	C
		OG1 THR B 485	35.425 39.830 54.489 1.00 38.41	0
		CG2 THR B 485	33.687 40.329 56.033 1.00 31.37	C
		N LEUB 486	36.455 42.687 57.410 1.00 40.70	N
		CA LEUB 486	36.524 43.442 58.661 1.00 39.17	C
		C LEUB 486	36.357 44.937 58.426 1.00 36.46	C
		O LEUB 486		0
		CB LEUB 486	37.819 43.240 59.397 1.00 37.63	C
		CG LEUB 486	37.839 42.538 60.735 1.00 39.49	C
		CD1 LEU B 486	36.471 42.392 61.383 1.00 40.00	C
		CD2 LEU B 486	38.533 41.180 60.628 1.00 35.73	C
ATOM	3191	N ILE B 487	37.092 45.487 57.475 1.00 37.80	N

			36.971 46.933 57.230 1.00 41.68	С
			35.587 47.346 56.741 1.00 40.87	C
ATOM		O ILEB 487		O
ATOM	3195	CB ILE B 487	38.025 47.395 56.224 1.00 40.44	С
ATOM		CG1 ILE B 487	•	С
ATOM			37.795 48.871 55.903 1.00 39.33	C
			39.851 48.181 57.775 1.00 41.18	С
ATOM	3199	N HISB 488		N
ATOM	3200	CA HIS B 488	33.689 46.702 55.338 1.00 47.90	С
ATOM		C HIS B 488	32.692 46.897 56.470 1.00 45.88	С
ATOM		O HISB 488		О
ATOM			33.346 45.498 54.470 1.00 50.31	С
ATOM		CG HIS B 488		С
ATOM		ND1 HIS B 488	30.859 44.934 54.302 1.00 57.87	N
			31.534 46.527 52.925 1.00 56.23	С
			29.809 45.323 53.611 1.00 58.24	С
		NE2 HIS B 488	30.211 46.273 52.783 1.00 58.77	N
		N LEUB 489		N
ATOM	3210	CA LEU B 489		С
		C LEU B 489		C
		O LEUB 489		0
		CB LEU B 489		С
		CG LEU B 489		С
			32.515 42.588 59.850 1.00 37.93	C
		CD2 LEU B 489		C
ATOM		N MET B 490		N
ATOM		CA MET B 490		C
ATOM		C MET B 490	33.001 50.287 59.363 1.00 44.69	C
ATOM		O MET B 490		0
ATOM		CB MET B 490	35.010 49.207 60.413 1.00 45.72	C
ATOM		CG MET B 490		C
		SD MET B 490		S
ATOM		CE MET B 490	37.054 46.523 62.575 1.00 44.78	C
		N ALA B 491	33.208 50.332 58.056 1.00 48.14	N
		CA ALA B 491	32.766 51.454 57.213 1.00 49.71	C
		C ALA B 491	31.248 51.491 57.282 1.00 55.03	C
		O ALA B 491	30.614 52.476 57.607 1.00 56.54	0
		CB ALA B 491	33.213 51.273 55.791 1.00 42.64	C
		N LYS B 492	30.681 50.309 57.031 1.00 59.07	N
		CA LYS B 492	29.233 50.124 57.088 1.00 61.88	C
		C LYS B 492	28.694 50.716 58.374 1.00 61.14	C
		O LYS B 492	27.738 51.490 58.326 1.00 65.25	0
		CB LYS B 492	28.912 48.648 56.973 1.00 65.85	C C
		CG LYS B 492	27.487 48.224 56.873 1.00 70.73	C
		CD LYS B 492	27.335 46.970 56.007 1.00 75.73	C
		CE LYS B 492	25.939 47.010 55.356 1.00 79.99	N
		NZ LYS B 492	25.382 45.631 55.150 1.00 83.64	
		N ALA B 493	29.300 50.465 59.505 1.00 59.06	N
ATOM	3240	CA ALA B 493	28.979 50.984 60.803 1.00 58.83	С

			29.194 52.493 60.929 1.00 60.61	С
			28.820 53.090 61.935 1.00 59.39	0
			29.902 50.311 61.828 1.00 58.13	С
		N GLY B 494		N
			30.149 54.469 59.878 1.00 62.54	С
		C GLY B 494		C
ATOM			31.413 56.184 60.897 1.00 66.15	0
			32.414 54.173 60.671 1.00 60.31	N
			33.613 54.731 61.339 1.00 55.79	С
		C LEU B 495		С
		O LEU B 495		О
			34.497 53.673 61.886 1.00 52.94	С
			34.054 52.508 62.694 1.00 50.03	С
			35.176 52.086 63.635 1.00 50.56	С
			32.772 52.721 63.431 1.00 48.72	С
		N THR B 496		N
		CA THR B 496		С
		C THR B 496		С
ATOM			37.224 55.107 59.559 1.00 57.11	0
		CB THR B 496		С
		OG1 THR B 496		0
			35.368 59.344 60.587 1.00 56.74	С
			37.732 56.636 58.027 1.00 56.81	N
			38.809 55.838 57.461 1.00 58.93	C
		C LEU B 497		C,
		O LEU B 497		0
			39.406 56.537 56.248 1.00 57.10	C
			38.864 55.921 54.946 1.00 60.97	C
			38.737 56.909 53.812 1.00 61.29	C
			39.749 54.735 54.590 1.00 61.42	C
			40.116 56.642 59.298 1.00 60.04	N
		CA GLN B 498		С
ATOM		C GLN B 498	40.655 55.619 61.429 1.00 56.58	C
		O GLN B 498	41.383 54.779 61.906 1.00 54.84	0
		CB GLN B 498	41.322 57.959 60.954 1.00 59.96	C
		CG GLN B 498	42.003 57.852 62.316 1.00 64.82	C
		CD GLN B 498	42.807 59.111 62.587 1.00 66.88	C
		OE1 GLN B 498	42.325 59.914 63.377 1.00 70.04	0
		NE2 GLN B 498	43.951 59.235 61.948 1.00 68.14	N
		N GLN B 499	39.387 55.786 61.796 1.00 56.24	N
		CA GLN B 499	38.822 54.914 62.829 1.00 56.35	С
		C GLN B 499	38.856 53.453 62.393 1.00 56.05	C
		O GLN B 499	39.074 52.610 63.264 1.00 57.20	0
		CB GLN B 499	37.424 55.348 63.149 1.00 55.66	C
		CG GLN B 499	37.327 56.721 63.773 1.00 56.83	C
		CD GLN B 499	35.871 56.986 64.130 1.00 58.69	C
	_	OE1 GLN B 499	35.006 56.866 63.274 1.00 58.39	0
		NE2 GLN B 499	35.642 57.324 65.385 1.00 61.19	N
ATOM	3289	N GLN B 500	38.623 53.155 61.132 1.00 52.26	N

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ATOM	3290	CA GLN B 500	38.721 51.832 60.580 1.00 48.06	
ATOM	3291	C GLN B 500	40.063 51.186 60.796 1.00 48.29	С
ATOM	3292	O GLN B 500	40.155 50.095 61.389 1.00 51.62	0
ATOM	3293	CB GLN B 500	38.513 51.894 59.041 1.00 45.29	C
ATOM	3294	CG GLN B 500	37.067 51.860 58.683 1.00 45.42	С
ATOM	3295	CD GLN B 500	36.618 52.564 57.441 1.00 45.44	С
ATOM	3296	OE1 GLN B 500	37.103 52.308 56.351 1.00 46.78	0
ATOM	3297	NE2 GLN B 500	35.648 53.468 57.589 1.00 44.47	N
ATOM	3298	N AHIS B 501	41.170 51.777 60.317 0.50 46.65	N
ATOM	3299	N BHIS B 501	41.099 51.854 60.328 0.50 47.93	N
ATOM	3300	CA AHIS B 501	42.463 51.100 60.524 0.50 43.55	С
ATOM	3301	CA BHIS B 501	42.477 51.385 60.430 0.50 46.45	С
ATOM	3302	C AHIS B 501	42.770 50.998 62.015 0.50 44.08	С
ATOM	3303	C BHIS B 501	42.918 51.257 61.881 0.50 45.96	С
ATOM	3304	O AHIS B 501	43.503 50.096 62.434 0.50 46.22	0
ATOM	3305	O BHIS B 501	43.586 50.264 62.211 0.50 47.87	0
ATOM	3306	CB AHIS B 501	43.619 51.724 59.805 0.50 41.42	С
ATOM	3307	CB BHIS B 501	43.367 52.356 59.651 0.50 47.09	С
ATOM	3308	CG AHIS B 501	43.981 53.129 60.147 0.50 40.96	С
ATOM	3309	CG BHIS B 501	43.020 52.436 58.188 0.50 48.40	С
ATOM	3310	ND1AHIS B 501	44.259 54.067 59.171 0.50 41.42	N
		ND1BHIS B 501	42.555 51.328 57.498 0.50 48.78	N
			44.121 53.774 61.328 0.50 40.78	С
			43.114 53.436 57.281 0.50 46.35	C
			44.534 55.223 59.764 0.50 43.40	С
		CE1BHIS B 501	42.368 51.660 56.234 0.50 48.60	С
ATOM	3316	NE2AHIS B 501	44.438 55.078 61.079 0.50 40.95	N
		NE2BHIS B 501	42.705 52.928 56.081 0.50 46.13	N
		N GLN B 502	42.228 51.930 62.808 1.00 42.77	N
		CA GLN B 502	42.557 51.941 64.220 1.00 40.75	C
		C GLN B 502		C
			42.647 50.028 65.601 1.00 36.67	0
		CB GLN B 502	42.252 53.228 64.935 1.00 38.57	C
		CG GLN B 502	43.059 54.353 64.298 1.00 40.97	C
		CD GLN B 502	43.087 55.565 65.193 1.00 42.76	C
		OE1 GLN B 502	44.039 56.323 65.007 1.00 49.28	0
		NE2 GLN B 502	42.164 55.761 66.094 1.00 42.12	N
		N ARG B 503	40.630 50.621 64.649 1.00 39.47	N
		CA ARG B 503	39.864 49.519 65.188 1.00 36.78	C
		C ARG B 503	40.427 48.201 64.642 1.00 34.42	C
		O ARGB 503	40.677 47.297 65.427 1.00 34.41	0
		CB ARG B 503	38.410 49.557 64.829 1.00 36.81	C
		CG ARG B 503	37.638 48.456 65.653 1.00 35.98	C
		CD ARG B 503	36.179 48.843 65.506 1.00 35.57	С
		NE ARG B 503		N
		CZ ARG B 503	34.997 47.930 67.391 1.00 42.50	C
		NH1 ARG B 503	35.680 48.835 68.083 1.00 44.65	N
		NH2 ARG B 503	34.169 47.071 67.944 1.00 43.19	N
ATOM	3338	N LEU B 504	40.726 48.172 63.368 1.00 32.25	N

ATOM 3339 CA LEU B 504 41.292 46.936 62.823 1.00 33.65 C 42.525 46.549 63.601 1.00 36.37 C ATOM 3340 C LEUB 504 0 42.718 45.361 63.937 1.00 38.64 ATOM 3341 O LEUB 504 41.649 47.125 61.351 1.00 32.77 C ATOM 3342 CB LEU B 504 42.329 45.917 60.688 1.00 28.02 ATOM 3343 CG LEU B 504 ATOM 3344 CD1 LEU B 504 41.351 44.779 60.549 1.00 20.13 C ATOM 3345 CD2 LEU B 504 42.931 46.378 59.373 1.00 23.43 43.388 47.540 63.857 1.00 37.99 ATOM 3346 N ALA B 505 N ATOM 3347 CA ALA B 505 44.651 47.278 64.606 1.00 31.73 C ATOM 3348 C ALA B 505 44.359 46.883 66.023 1.00 29.70 C ATOM 3349 O ALA B 505 44.932 45.965 66.578 1.00 26.36 0 ATOM 3350 CB ALA B 505 45.503 48.523 64.577 1.00 32.14 C 43.415 47.597 66.669 1.00 33.66 ATOM 3351 N GLN B 506 N C ATOM 3352 CA GLN B 506 43.046 47.218 68.038 1.00 35.30 ATOM 3353 C GLN B 506 42.616 45.755 68.063 1.00 36.27 C ATOM 3354 O GLN B 506 43.246 45.000 68.820 1.00 39.25 O ATOM 3355 CB GLN B 506 41.990 48.086 68.669 1.00 35.30 C 42,394 49,533 68,813 1,00 39,85 ATOM 3356 CG GLN B 506 41.214 50.474 68.812 1.00 45.28 ATOM 3357 CD GLN B 506 40.128 50.163 69.315 1.00 49.60 ATOM 3358 OE1 GLN B 506 ATOM 3359 NE2 GLN B 506 41.392 51.660 68.253 1.00 49.18 N ATOM 3360 N LEUB 507 41.690 45.322 67.198 1.00 32.30 N ATOM 3361 CA LEUB 507 41.346 43.911 67.223 1.00 30.88 C 42.491 42.993 66.935 1.00 29.84 ATOM 3362 C LEUB 507 C 42.616 41.987 67.596 1.00 31.13 O ATOM 3363 O LEUB 507 ATOM 3364 CB LEUB 507 40.259 43.609 66.138 1.00 32.27 39.091 44.575 66.311 1.00 33.70 ATOM 3365 CG LEUB 507 ATOM 3366 CD1 LEU B 507 38.048 44.471 65.247 1.00 34.24 38.559 44.294 67.697 1.00 35.31 C ATOM 3367 CD2 LEU B 507 43.350 43.211 65.930 1.00 31.10 N ATOM 3368 N LEUB 508 ATOM 3369 CA LEU B 508 44,400 42,227 65,712 1,00 30,54 C C ATOM 3370 C LEU B 508 45.435 42.214 66.800 1.00 30.57 ATOM 3371 O LEUB 508 45.928 41.097 66.978 1.00 33.14 0 ATOM 3372 CB LEU B 508 45.035 42.228 64.339 1.00 29.19 ATOM 3373 CG LEU B 508 43.984 42.309 63.217 1.00 30.62 ATOM 3374 CD1 LEU B 508 44.677 42.905 62.014 1.00 31.84 C ATOM 3375 CD2 LEU B 508 43.354 40.958 63.003 1.00 26.58 ATOM 3376 N LEUB 509 45.638 43.235 67.613 1.00 28.82 N 46.620 43.082 68.682 1.00 27.22 ATOM 3377 CA LEUB 509 C C ATOM 3378 C LEU B 509 46.035 42.165 69.719 1.00 30.73 ATOM 3379 O LEUB 509 46.837 41.469 70.369 1.00 32.94 0 ATOM 3380 CB LEU B 509 47.031 44.405 69.286 1.00 29.04 47.727 45.304 68.242 1.00 28.79 ATOM 3381 CG LEU B 509 C ATOM 3382 CD1 LEU B 509 48.237 46.507 68.932 1.00 35.11 ATOM 3383 CD2 LEU B 509 48.860 44,511 67.641 1.00 28.05 44.709 42.129 69.838 1.00 30.11 ATOM 3384 N ILE B 510 N ATOM 3385 CA ILE B 510 44.065 41.203 70.781 1.00 30.61 C 44.378 39.793 70.326 1.00 30.81 C ATOM 3386 C ILE B 510 44.466 38.844 71.147 1.00 32.18 0 ATOM 3387 O ILE B 510

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ATOM	3388 CB ILE B 510	42.576 41.539 70.920 1.00 35.88	C	
ATOM	3389 CG1 ILE B 510	42.321 42.740 71.838 1.00 39.34	С	
ATOM	3390 CG2 ILE B 510	41.722 40.376 71.437 1.00 34.95		
	3391 CD1 ILE B 510	40.870 43.207 71.863 1.00 39.83		
	3392 N LEUB 511		N	
		45.034 38.192 68.643 1.00 28.74		
		46.368 37.876 69.273 1.00 30.01	С	
		46.433 36.716 69.732 1.00 35.16	0	
		45.001 37.896 67.156 1.00 26.69		
		43.616 38.137 66.479 1.00 26.06	С	
		43.726 37.691 65.044 1.00 16.51	C	
	3399 CD2 LEU B 511		С	
	3400 N SER B 512		N	
		48.520 38.200 70.312 1.00 31.98	C	
		48.256 37.766 71.742 1.00 30.82	C	
		48.933 36.829 72.224 1.00 30.49	0	
		49.652 39.244 70.422 1.00 35.44	C	
		49.319 40.233 69.447 1.00 46.47	0	
	3406 N HIS B 513		N	
		47.015 38.093 73.790 1.00 32.67	C	
	3408 C HIS B 513	· ·	C	
	3409 O HIS B 513	46.643 35.820 74.605 1.00 32.52 46.062 39.120 74.347 1.00 34.61	O C	
		46.660 40.486 74.389 1.00 37.60	C	
ATOM	2411 CO 1113 B 213	40.000 40.480 74.389 1.00 37.00		
ATOM	2412 CD2 HIS B 513	47.777 40.752 75.169 1.00 41.78 46.307 41.641 73.838 1.00 42.38	C	
ATOM	3414 CE1 HIS B 513	48.086 42.014 75.057 1.00 44.76	Č	
		47.216 42.599 74.230 1.00 47.20	N	
	3416 N ILE B 514		N	
		44.770 35.276 72.708 1.00 33.15	Ċ	
	3418 C ILE B 514		C	
	3419 O ILEB 514	45.878 33.229 73.224 1.00 34.97	0	
	3420 CB ILE B 514	43.635 35.391 71.710 1.00 32.90	C	
	3421 CG1 ILE B 514	42.445 36.115 72.387 1.00 29.27	C	
	3422 CG2 ILE B 514	43.169 34.033 71.236 1.00 34.89	С	
	3423 CD1 ILE B 514	41.575 36.805 71.391 1.00 32.54	C .	
	3424 N ARG B 515	46.768 34.357 71.566 1.00 32.82	N	
ATOM	3425 CA ARG B 515	47.815 33.347 71.392 1.00 30.13	С	
ATOM	3426 C ARG B 515	48.528 33.144 72.713 1.00 30.92	С	
ATOM	3427 O ARG B 515	48.779 32.095 73.242 1.00 32.38	0	
ATOM	3428 CB ARG B 515	48.787 33.853 70.351 1.00 32.12	С	
	3429 CG ARG B 515	50.056 33.038 70.203 1.00 32.29	С	
	3430 CD ARG B 515	49.706 31.820 69.408 1.00 35.87	С	
	3431 NE ARG B 515	50.513 31.578 68.211 1.00 39.98	N	
	3432 CZ ARG B 515	50.021 31.993 67.036 1.00 43.57	С	
	3433 NH1 ARG B 515		N	
	3434 NH2 ARG B 515		N	
	3435 N HIS B 516	48.861 34.252 73.371 1.00 33.83	N	
ATOM	3436 CA HIS B 516	49.522 34.215 74.650 1.00 31.88	С	

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			С
			0
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			C
3443 CE1	HIS B 516	52.531 35.272 77.481 1.00 35.00	С
			N
3445 N N	MET B 517	47.455 33.591 75.850 1.00 31.17	N
3446 CA	MET B 517		C
3447 C N	MET B 517	46.685 31.324 76.296 1.00 30.07	С
			Ο
3449 CB	MET B 517	45.242 33.276 76.730 1.00 32.23	С
3450 CG	MET B 517	45.217 34.646 77.408 1.00 31.26	С
3451 SD 1	MET B 517	43.573 35.270 77.608 1.00 37.21	S
3452 CE 1	MET B 517	43.181 35.765 75.937 1.00 28.84	C
3453 N S	ER B 518	46.527 31.089 74.977 1.00 30.90	N
3454 CA	SER B 518	46.600 29.676 74.543 1.00 31.77	С
3455 C S	ER B 518	47.939 29.094 74.903 1.00 31.54	С
3456 O S	ER B 518	48.073 28.045 75.505 1.00 33.26	Ο
3457 CB :	SER B 518	46.369 29.547 73.033 1.00 32.22	C
3458 OG	SER B 518	46.480 28.189 72.666 1.00 29.39	Ο
3459 N A	SN B 519	49.028 29.748 74.511 1.00 32.87	N
3460 CA	ASN B 519	50.339 29.190 74.896 1.00 35.57	C
3461 C A	SN B 519	50.367 28.942 76.372 1.00 39.13	C
3462 O A	SN B 519	50.678 27.857 76.863 1.00 41.01	Ο
3463 CB	ASN B 519	51.430 30.134 74.396 1.00 33.23	С
3464 CG			C
3465 OD1	ASN B 519	51.665 30.870 72.076 1.00 38.85	О
			N
			N
			С
			С
			Ο
			C
			С
			С
			С
			N
			N
			С
			С
3479 O G	LY B 521	47.258 25.105 79.160 1.00 38.25	0
		48.115 25.848 77.306 1.00 42.81	N
		48.619 24.507 76.999 1.00 45.50	С
			С
			0
	MET B 522	49.239 24.413 75.630 1.00 40.58	С
3485 CG I	MET B 522	48.145 24.744 74.627 1.00 43.42	С
	3438 O F 3439 CB 3440 CG 3441 ND1 3442 CD2 3443 CE1 3444 NE2 3445 N N 3446 CA 3447 C N 3448 O N 3449 CB 3450 CG 3451 SD N 3452 CE N 3453 N S 3454 CA 3455 C S 3456 O S 3457 CB N 3458 OG 3457 CB N 3460 CA 3461 C A 3462 O A 3463 CB N 3460 CA 3461 C A 3462 O A 3463 CB N 3460 CA 3461 C A 3462 O A 3463 CB N 3460 CA 3461 C A 3462 O A 3463 CB N 3460 CA 3461 C A 3462 O A 3463 CB N 3460 CA 3461 C A 3462 O A 3463 CB N 3460 CA 3461 C A 3462 O A 3463 CB N 3460 CA 3461 C A 3462 O A 3463 CB N 3460 CA 3461 C A 3462 O A 3463 CB N 3460 CA 3461 C A 3462 O A 3463 CB N 3460 CA 3461 C A 3462 C A 3463 CB N 3460 CA 3461 CB N	3438 O HIS B 516 3439 CB HIS B 516 3440 CG HIS B 516 3441 ND1 HIS B 516 3442 CD2 HIS B 516 3443 CE1 HIS B 516 3444 NE2 HIS B 516 3445 N MET B 517 3446 CA MET B 517 3446 CA MET B 517 3447 C MET B 517 3448 O MET B 517 3450 CG MET B 517 3451 SD MET B 517 3451 SD MET B 517 3452 CE MET B 518 3454 CA SER B 518 3455 C SER B 518 3456 O SER B 518 3457 CB SER B 518 3458 OG SER B 518 3459 N ASN B 519 3460 CA ASN B 519 3461 C ASN B 519 3462 O ASN B 519 3463 CB ASN B 519 3464 CG ASN B 519 3465 OD1 ASN B 519 3466 ND2 ASN B 519 3467 N LYS B 520 3476 N CYS B 520 3470 O LYS B 520 3471 CB LYS B 520 3471 CB LYS B 520 3472 CG LYS B 520 3474 CE LYS B 520 3475 NZ LYS B 520 3476 N GLY B 521 3477 CA GLY B 521 3478 C GLY B 521 3479 O GLY B 521 3479 CA MET B 522 3481 CA MET B 522 3483 O MET B 522	3438 O HIS B 516 3439 CB HIS B 516 3440 CG HIS B 516 3441 ND1 HIS B 516 3442 CD2 HIS B 516 3442 CD2 HIS B 516 3443 CEI HIS B 516 3444 NE2 HIS B 516 3444 NE2 HIS B 516 3445 N MET B 517 3446 CA MET B 517 3446 CA MET B 517 3447 C MET B 517 3448 O MET B 517 3449 CB MET B 517 3450 CG MET B 517 3451 SD MET B 517 3452 CE MET B 517 3453 N SER B 518 3454 CA SER B 518 3455 C SER B 518 3455 C SER B 518 3456 O SER B 518 3456 O SER B 518 3457 CB SER B 518 3458 OG SER B 518 3459 N ASN B 519 3460 CA ASN B 519 3461 C ASN B 519 3462 O ASN B 519 3463 CB ASN B 519 3466 ND2 ASN B 519 3466 ND2 ASN B 519 3467 N LYS B 520 3468 CA LYS B 520 3470 O LYS B 520 3471 CB LYS B 520 3472 CG LYS B 520 3473 CD LYS B 520 3474 CE LYS B 520 3475 NZ LYS B 520 3476 N GLY B 521 3477 CA GLY B 521 3480 N MET B 522 3481 CA MET B 522 3484 CB MET B 522 3486 CA MET B 522 3486 CA MET B 522 3484 CB MET B 522 3487 O MET B 522 3487 O MET B 522 3488 CB MET B 522 3488 CB MET B 522 3488 CB MET B 522 3484 CB MET B 522 3486 CB MIS B 522 3486 CB MIS B 522 3486 CB MET B 522 3487 CB MIS S 516 50.758 35.76 76.328 1.00 33.20 36.045 77.616 1.00 37.42 35.00 37.72 36.045 77.616 1.00 37.42 36.045 77.616 1.00 30.07 36.045 77.616 1.00 30.07 36.045 77.616 1.00 30.07 36.045 77.616 1.00 30.07 36.045 77.616 1.00 30.07 36.045 77.616 1.00 30.07 36.045 77.608 1.00 30.07 36.045 77.608 1.00 30.07 36.045 77.608 1.00 30.07 36.045 77.616 1.00 30.07 36.057 77.608 1.00 30.22 37.70 76.08 1.00 30.22 37.70 76.08 1.00 30.22 37.70 76.08 1.00 30.22 37.70 76.08 1.00 30.22 37.70 76.08 1.00 30.22 37.70 76.08 1.00 30.22 37

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ATOM	3486 SD MET B 522 48.718 24.184 73.023 1.00 48.	78 S
	3487 CE MET B 522 47.330 24.747 72.036 1.00 46.	57 C
	3488 N GLU B 523 50.529 24.985 78.435 1.00 56.2	
	3489 CA GLUB 523 51.544 24.685 79.459 1.00 59.	
	3490 C GLU B 523 50.800 24.081 80.664 1.00 61.3	
	3491 O GLU B 523 51.112 23.012 81.125 1.00 62.0	
	3492 CB GLUB 523 52.236 25.939 79.934 1.00 60.6	
ATOM	3493 CG GLUB 523 53.692 26.141 80.004 1.00 62.	32 C
ATOM	3494 CD GLUB 523 54.189 27.545 79.761 1.00 65.4 3495 OE1 GLUB 523 54.319 28.008 78.588 1.00 68.	44 C
ATOM	3495 OE1 GLU B 523 54.319 28.008 78.588 1.00 68.	32 0
	3496 OE2 GLU B 523 54.460 28.254 80.746 1.00 66.	
	3497 N HIS B 524 49.819 24.808 81.137 1.00 65.14	
	3498 CA HIS B 524 48.998 24.437 82.275 1.00 69.7	
ATOM	3499 C HIS B 524 48.255 23.145 82.016 1.00 69.68	C
ATOM	3500 O HIS B 524 48.273 22.235 82.845 1.00 67.93	0
ATOM	3501 CB HIS B 524 48.048 25.598 82.574 1.00 73.3	4 C
	3502 CG HIS B 524 47.051 25.312 83.628 1.00 77.4	
ATOM	3503 ND1 HIS B 524 45.809 25.918 83.647 1.00 79.8	32 N
ATOM	3504 CD2 HIS B 524 47.105 24.488 84.700 1.00 79.3	32 C
ATOM	3505 CE1 HIS B 524 45.125 25.493 84.701 1.00 80.7 3506 NE2 HIS B 524 45.894 24.624 85.344 1.00 82.5	3 C
ATOM	3500 NE2 HIS B 324	59 N 8 N
	3507 N LEUB 525 47.715 22.983 80.812 1.00 70.58 3508 CA LEUB 525 47.028 21.725 80.538 1.00 74.8	
	3508 CA LEU B 525 47.028 21.725 80.538 1.00 74.6	
	3510 O LEUB 525 47.759 19.633 81.377 1.00 81.4	
	3511 CB LEU B 525 46.341 21.724 79.198 1.00 73.4	
	3512 CG LEU B 525 44.836 21.743 79.060 1.00 71.1	
	3513 CD1 LEU B 525 44.148 22.671 80.045 1.00 70.	
	3514 CD2 LEU B 525 44.459 22.156 77.636 1.00 71.	
	3515 N TYR B 526 49.165 20.643 79.958 1.00 84.7	
	3516 CA TYR B 526 50.153 19.579 80.005 1.00 91.0	
	3517 C TYR B 526 50.835 19.399 81.335 1.00 92.4	
	3518 O TYR B 526 51.138 18.252 81.737 1.00 92.7	
	3519 CB TYR B 526 51.147 19.722 78.849 1.00 95.7	
	3520 CG ATYR B 526 50.422 19.566 77.521 0.50 97	
	3521 CG BTYR B 526 52.174 18.632 78.708 0.50 98	
	3522 CD1ATYR B 526 50.194 18.307 76.984 0.50 98	
ATOM	3523 CD1BTYR B 526 52.083 17.432 79.396 0.5010	0.15 C
ATOM	3524 CD2ATYR B 526 49.922 20.658 76.836 0.50 98	
ATOM	3525 CD2BTYR B 526 53.272 18.779 77.859 0.50 99	
ATOM	3526 CE1ATYR B 526 49.514 18.159 75.788 0.50 99	
	3527 CE1BTYR B 526 53.002 16.422 79.294 0.5010	
	3528 CE2ATYR B 526 49.239 20.528 75.647 0.50 99	
	3529 CE2BTYR B 526 54.213 17.772 77.733 0.5010	
	3530 CZ ATYR B 526 49.040 19.268 75.129 0.50 99.	
	3531 CZ BTYR B 526 54.075 16.603 78.446 0.50101	
	3532 OH ATYR B 526 48.354 19.121 73.949 0.50100	
	3533 OH BTYR B 526 55.016 15.607 78.310 0.50103	
ATOM	3534 N SER B 527 50.986 20.432 82.151 1.00 93.82	2 N

51.517 20.212 83.504 1.00 96.43 C ATOM 3535 CA SER B 527 ATOM 3536 C SER B 527 50.635 19.206 84.243 1.00 99.93 C ATOM 3537 O SER B 527 51.122 18.212 84.783 1.00 99.91 0 C 51.654 21.528 84.228 1.00 95.12 ATOM 3538 CB SER B 527 50.575 21.842 85.055 1.00 93.84 0 ATOM 3539 OG SER B 527 49.324 19.442 84.235 1.00104.05 ATOM 3540 N MET B 528 48.348 18.580 84.874 1.00106.28 C ATOM 3541 CA MET B 528 ATOM 3542 C MET B 528 48.514 17.114 84.501 1.00109.30 0 ATOM 3543 O MET B 528 49.146 16.375 85.280 1.00110.26 ATOM 3544 CB MET B 528 46.934 19.066 84.578 1.00104.92 C C ATOM 3545 CG MET B 528 46.616 20.428 85.186 1.00103.89 S ATOM 3546 SD MET B 528 45.067 21.090 84.521 1.00102.69 C ATOM 3547 CE MET B 528 43.976 19.685 84.768 1.00103.03 ATOM 3548 N LYS B 529 47.979 16.659 83.392 1.00112.58 N ATOM 3549 CA LYS B 529 47.968 15.274 82.952 1.00114.66 C C ATOM 3550 C LYS B 529 46.519 14.757 82.954 1.00115.44 ATOM 3551 O LYS B 529 46.210 13.626 83.307 1.00115.58 0 48.833 14.322 83.758 1.00115.06 C ATOM 3552 CB LYS B 529 47.047 14.467 69.426 1.00 90.47 ATOM 3553 N LEUB 536 N ATOM 3554 CA LEUB 536 45.800 15.110 68.992 1.00 91.19 C ATOM 3555 C LEUB 536 45.806 15.246 67.479 1.00 90.41 C ATOM 3556 O LEUB 536 44.762 15.397 66.845 1.00 91.34 0 45,635 16.485 69.635 1.00 90.56 C ATOM 3557 CB LEUB 536 C 44.545 17.411 69.144 1.00 89.27 ATOM 3558 CG LEUB 536 ATOM 3559 CD1 LEU B 536 43.162 16.805 69.074 1.00 89.56 C C 44,632 18,761 69,813 1,00 88,59 ATOM 3560 CD2 LEU B 536 ATOM 3561 N TYR B 537 47.016 15.149 66.935 1.00 91.03 N C 47.194 15.255 65.492 1.00 91.03 ATOM 3562 CA TYR B 537 C ATOM 3563 C TYR B 537 46.231 14.307 64.787 1.00 90.74 ATOM 3564 O TYR B 537 45.467 14.712 63.911 1.00 89.89 0 ATOM 3565 CB TYR B 537 48.651 14.949 65.101 1.00 90.58 C C ATOM 3566 CG TYR B 537 48,832 15.074 63.601 1.00 91.36 C 48.486 14.030 62.760 1.00 91.31 ATOM 3567 CD1 TYR B 537 C 49.323 16.251 63.041 1.00 92.16 ATOM 3568 CD2 TYR B 537 48.636 14.149 61.396 1.00 93.25 C ATOM 3569 CE1 TYR B 537 C 49.481 16.379 61.672 1.00 92.69 ATOM 3570 CE2 TYR B 537 C ATOM 3571 CZ TYR B 537 49.134 15.324 60.855 1.00 93.50 O 49.265 15.403 59.485 1.00 93.62 ATOM 3572 OH TYR B 537 46.306 13.033 65.173 1.00 91.50 N ATOM 3573 N ASP B 538 45.486 11.989 64.559 1.00 92.46 C ATOM 3574 CA ASP B 538 C ATOM 3575 C ASP B 538 44.045 12.098 65.027 1.00 89.47 ATOM 3576 O ASP B 538 43.116 11.887 64.239 1.00 89.78 O C ATOM 3577 CB ASP B 538 46.059 10.611 64.812 1.00 96.58 C ATOM 3578 CG ASP B 538 47,466 10.656 65.393 1.00 98.56 48,385 11.085 64.658 1.00 98.61 0 ATOM 3579 OD1 ASP B 538 ATOM 3580 OD2 ASP B 538 47.567 10.262 66.578 1.00100.00 0 N ATOM 3581 N LEUB 539 43.860 12.515 66.285 1.00 85.65 C ATOM 3582 CA LEUB 539 42.515 12.744 66.774 1.00 82.51 C 41.753 13.616 65.771 1.00 79.45 ATOM 3583 C LEUB 539

103/371 LEU B 539 40 699 13 13 13

			6 1 THE T 10	40 (00 10 107 (5 351 1 00 77 06	0
				40.688 13.197 65.351 1.00 77.96	0
				42.444 13.387 68.160 1.00 83.22	C C
				40.995 13.548 68.674 1.00 84.94	
	MOTA		-	40.178 12.277 68.459 1.00 84.31	C
				40.886 13.991 70.123 1.00 84.23	C
				42.333 14.748 65.377 1.00 76.53	N
				41.691 15.629 64.394 1.00 74.04	C
				41.634 15.010 63.008 1.00 72.97	C
				40.703 15.130 62.207 1.00 67.85	О
				42.448 16.976 64.343 1.00 69.75	С
				42.627 17.636 65.710 1.00 67.68	С
				43.630 18.774 65.641 1.00 67.75	С
A	MOTA	3596	CD2 LEU B 540	41.288 18.127 66.240 1.00 66.55	С
A	MOTA	3597	N LEUB 541	42.734 14.308 62.684 1.00 74.85	N
F	MOTA	3598	CA LEUB 541	42.817 13.660 61.369 1.00 75.55	С
A	MOTA	3599	C LEU B 541	41.604 12.757 61.179 1.00 74.33	С
ŀ	MOTA	3600	O LEU B 541	40.915 12.818 60.174 1.00 73.71	Ο
A	MOTA	3601	CB LEUB 541	44.101 12.859 61.270 1.00 76.52	С
1	MOTA	3602	CG LEUB 541	44.429 12.193 59.942 1.00 77.83	С
	MOTA			43.682 12.832 58.761 1.00 77.63	С
				45.937 12.242 59.708 1.00 76.18	С
				41.323 11.945 62.184 1.00 74.70	Ν
				40.161 11.055 62.111 1.00 78.10	С
,	ATOM	3607	C GLUB 542	38.871 11.830 62.028 1.00 76.88	С
	ATOM			38.025 11.609 61.165 1.00 76.15	0
	ATOM			40.206 10.099 63.314 1.00 81.69	С
	ATOM			41.236 8.981 63.062 1.00 86.31	С
				40.967 8.283 61.729 1.00 90.86	Ċ
				39.878 7.669 61.534 1.00 92.07	0
				41.868 8.367 60.853 1.00 92.44	0
				38.753 12.820 62.890 1.00 76.90	N
				37.654 13.758 62.973 1.00 77.35	C
	ATOM			37.421 14.492 61.665 1.00 76.40	C
				36.317 14.683 61.196 1.00 73.90	Ö
			CB MET B 543	38.008 14.769 64.083 1.00 79.63	C
			CG MET B 543	38.041 14.163 65.465 1.00 80.33	č
				37.001 15.039 66.655 1.00 83.37	S
			SD MET B 543	38.090 14.960 68.082 1.00 80.57	C
			CE MET B 543		N
			N LEUB 544	38.514 14.931 61.037 1.00 78.72	C
			CA LEUB 544	38.450 15.633 59.761 1.00 80.40	
			C LEUB 544	38.116 14.649 58.643 1.00 86.77	С
	ATOM		O LEUB 544	37.409 14.973 57.688 1.00 85.08	0
			CB LEUB 544	39.762 16.355 59.539 1.00 75.21	C
			CG LEUB 544	39.822 17.785 60.068 1.00 72.72	C
			CD1 LEU B 544	41.249 18.270 60.143 1.00 70.71	C
			CD2 LEU B 544	38.970 18.702 59.200 1.00 72.37	C
			N ASP B 545	38.582 13.412 58.826 1.00 94.59	N
	ATOM		CA ASP B 545	38.296 12.264 57.997 1.00101.77	C
4	ATOM	3632	C ASP B 545	36.804 11.881 58.061 1.00103.94	С

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			104/371	
ATOM	3633	O ASP B 545	36.101 11.897 57.058 1.00103.96	0
		CB ASP B 545	39.074 11.042 58.483 1.00104.99	С
		CG ASP B 545	40.217 10.526 57.666 1.00107.94	С
		OD1 ASP B 545	40.367 10.845 56.456 1.00109.53	0
		OD2 ASP B 545	41.032 9.741 58.242 1.00107.92	Ο
		N ALA B 546	36.369 11.557 59.271 1.00106.70	N
ATOM	3639	CA ALA B 546	35.015 11.150 59.581 1.00110.47	С
ATOM	3640	C ALA B 546	33.945 12.129 59.146 1.00112.92	С
ATOM		O ALA B 546	32.865 11.719 58.724 1.00113.22	0
			34.881 10.866 61.078 1.00110.18	С
		N HIS B 547	34.213 13.420 59.155 1.00116.65	N
			33.322 14.479 58.740 1.00119.67	С
		C HIS B 547	32.766 14.292 57.336 1.00123.33	С
		O HIS B 547	31.663 14.755 57.030 1.00123.70	0
		CB HIS B 547	34.086 15.813 58.802 1.00118.14	С
			33.193 17.007 58.672 1.00116.79	С
			33.295 17.920 57.648 1.00115.21	N
			32.171 17.422 59.467 1.00116.21	С
		CE1 HIS B 547	32.379 18.843 57.812 1.00115.15	С
		NE2 HIS B 547	31.683 18.573 58.905 1.00115.69	N
		N ARG B 548		N
		CA ARG B 548	33.142 13.329 55.105 1.00132.03	С
		C ARG B 548	32.277 12.070 55.013 1.00134.33	C
		O ARG B 548	31.802 11.729 53.929 1.00134.94	0
		CB ARG B 548	34.396 13.180 54.235 1.00131.91	C
		N LEUB 549	32.074 11.401 56.138 1.00136.47	N
		CA LEUB 549	31.213 10.236 56.250 1.00138.06	C C
		C LEUB 549	30.140 10.461 57.323 1.00138.50	0
		O LEUB 549	29.531 9.529 57.840 1.00139.19	C
		CB LEU B 549 N HIS B 550	32.012 8.971 56.538 1.00138.52 29.921 11.734 57.655 1.00138.06	N
		CA HIS B 550	28.939 12.136 58.640 1.00137.04	C
			27.656 12.584 57.943 1.00138.03	c
			27.711 13.069 56.810 1.00139.03	Ö
			29.418 13.280 59.535 1.00134.98	C
		CG HIS B 550		Č
			30.606 13.616 61.734 1.00131.99	N
		CD2 HIS B 550		Ċ
		CE1 HIS B 550		Č
			31.180 11.617 62.283 1.00132.12	N
			26.545 12.411 58.645 1.00138.08	N
			25.256 12.796 58.080 1.00138.49	С
		C ALA B 551		С
			25.318 15.156 57.901 1.00139.61	0
			24.215 11.761 58.460 1.00139.09	С
TER				
			1 50.363 23.182 66.508 1.00 70.74	С
			1 50.898 24.501 67.006 1.00 63.90	С
			1 50.120 23.220 65.205 1.00 71.38	0

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1777 1771 2601 00 CD14D 201	50.159 22.259 67.288 1.00 73.88 O
HETATM 3691 O2 CBM B 381	
HETATM 3692 C1 RAL B 600	
HETATM 3693 C2 RAL B 600	36.077 25.070 77.112 1.00 39.83 C
HETATM 3694 C3 RAL B 600	35.957 26.328 76.578 1.00 38.16 C
HETATM 3695 O3 RAL B 600	34.871 26.528 75.754 1.00 40.43 O
HETATM 3696 C4 RAL B 600	36.882 27.310 76.907 1.00 39.29 C
HETATM 3697 C5 RAL B 600	37.925 27.033 77.738 1.00 39.54 C
HETATM 3698 S6 RAL B 600	39.146 28.022 78.355 1.00 40.30 S
HETATM 3699 C7 RAL B 600	39.970 26.805 79.208 1.00 41.19 C
HETATM 3700 C8 RAL B 600	41.199 27.019 80.019 1.00 39.95 C
HETATM 3701 C9 RAL B 600	41.345 28.185 80.728 1.00 41.84 C
HETATM 3702 C10 RAL B 600	42.438 28.411 81.548 1.00 44.69 C
HETATM 3703 C11 RAL B 600	43.437 27.448 81.612 1.00 45.99 C
HETATM 3704 O11 RAL B 600	44.521 27.695 82.432 1.00 50.33 O
HETATM 3705 C12 RAL B 600	43.314 26.290 80.885 1.00 42.47 C
HETATM 3706 C13 RAL B 600	42.179 26.085 80.108 1.00 39.90 C
HETATM 3707 C14 RAL B 600	38.054 25.738 78.252 1.00 38.16 C
HETATM 3708 C15 RAL B 600	39.227 25.613 79.090 1.00 38.60 C
HETATM 3709 C16 RAL B 600	39.540 24.434 79.718 1.00 37.47 C
HETATM 3710 O16 RAL B 600	39.634 24.372 80.932 1.00 36.58 O
HETATM 3711 C17 RAL B 600	39.914 23.230 78.994 1.00 34.13 C
HETATM 3712 C18 RAL B 600	39.972 22.094 79.765 1.00 34.98 C
HETATM 3713 C19 RAL B 600	40.396 20.876 79.214 1.00 34.59 C
HETATM 3714 C20 RAL B 600	40.771 20.895 77.901 1.00 38.96 C
HETATM 3715 C21 RAL B 600	40.752 22.057 77.116 1.00 37.83 C
HETATM 3716 C22 RAL B 600	40.305 23.245 77.679 1.00 35.52 C
HETATM 3717 O23 RAL B 600	41.204 19.791 77.200 1.00 44.41 O
HETATM 3718 C24 RAL B 600	40.319 18.706 77.123 1.00 45.36 C
HETATM 3719 C25 RAL B 600	41.196 17.625 76.411 1.00 44.46 C
HETATM 3720 N26 RAL B 600	40.895 17.562 74.984 1.00 43.60 N
HETATM 3721 C27 RAL B 600	41.659 16.562 74.294 1.00 43.45 C
HETATM 3722 C28 RAL B 600	41.488 16.507 72.779 1.00 44.58 C
HETATM 3723 C29 RAL B 600	
HETATM 3724 C30 RAL B 600	40.388 18.722 72.842 1.00 45.78 C
HETATM 3725 C31 RAL B 600	
	3.671 45.635 73.728 1.00 18.41
	5.939 43.852 69.249 1.00 23.40
	7.879 41.641 69.144 1.00 32.98
	2.161 43.516 68.328 1.00 32.96
	5.293 41.236 55.063 1.00 36.48
	0.117 45.566 50.606 1.00 44.30
_	5.937 34.473 57.692 1.00 38.73
-	0.523 44.664 70.139 1.00 37.12
	5.684 41.492 67.111 1.00 46.69
	2.332 42.566 71.041 1.00 48.09
	77.230 47.810 75.360 1.00 41.93
	8.753 44.504 65.387 1.00 47.61
	6.079 37.937 81.002 1.00 48.27
HETATM 14 O HOH 14 7	0.480 45.943 67.468 1.00 53.17

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106/371 56,336 35,571 76,185 1,00 44,22 HETATM 15 O HOH 15 40.293 54.526 68.285 1.00 65.88 HETATM 16 O HOH 16 48.191 42.643 49.929 1.00 66.50 HETATM 17 O HOH 17 HETATM 18 O HOH 42.953 57.811 69.507 1.00 88.95 18 **НЕТАТМ 19 О НОН** 19 66.169 45.843 67.240 1.00 30.54 20 63,477 52,158 67.006 1.00 37.54 HETATM 20 O HOH HETATM 21 O HOH 21 79.511 32.798 62.361 1.00 58.45 HETATM 22 O HOH 22 79,665 44,463 70,700 1,00 50,89 HETATM 23 O HOH 23 59.043 57.930 76.285 1.00 75.57 60.390 37.277 84.122 1.00 43.42 HETATM 24 O HOH 24 HETATM 25 O HOH 25 76.899 29.211 59.311 1.00 72.06 53.280 40.076 69.802 1.00 43.07 HETATM 26 O HOH 26 HETATM 27 O HOH 27 45,293 51,300 66,697 1,00 40,03 47.486 57.944 58.839 1.00 56.99 HETATM 28 O HOH 28 HETATM 29 O HOH 29 47.155 44.689 45.733 1.00 81.53 48.375 39.816 66.498 1.00 50.55 HETATM 30 O HOH 30 HETATM 31 O HOH 31 54.862 44.533 76.824 1.00 38.59 81,320 34,485 67,792 1.00 53.56 HETATM 32 O HOH 32 HETATM 33 O HOH 78.189 37.052 73.346 1.00 55.28 33 59.058 38.545 75.613 1.00 27.41 HETATM 34 O HOH 34 HETATM 35 O HOH 35 56.115 30.116 78.032 1.00 64.88 48.376 56.369 48.335 1.00 74.84 HETATM 36 O HOH 36 45.334 56.547 54.616 1.00 51.79 HETATM 37 O HOH 37 HETATM 38 O HOH 68.751 46.528 72.429 1.00 61.72 38 HETATM 39 O HOH 68.749 48.138 63.262 1.00 75.75 39 HETATM 40 O HOH 40 71.042 50.167 64.313 1.00 57.30 HETATM 41 O HOH 51.867 54.038 84.504 1.00 55.62 41 HETATM 42 O HOH 42 46.423 34.649 68.035 1.00 59.90 43 65.977 46.032 71.358 1.00 39.14 HETATM 43 O HOH HETATM 44 O HOH 51.878 43.672 50.996 1.00 56.18 44 HETATM 45 O HOH 45 80.471 31.343 76.488 1.00 42.36 71.303 44.041 59.439 1.00 70.71 HETATM 46 O HOH 46 41.452 53.507 71.888 1.00 75.54 HETATM 47 O HOH 47 HETATM 48 O HOH 48 82.937 41.654 71.088 1.00 75.67 HETATM 49 O HOH 65,172 34,557 81.617 1.00 57.84 49 HETATM 50 O HOH 50 67.048 50.080 60.811 1.00 49.02 HETATM 51 O HOH 51 55,298 50,332 52,676 1,00 48,09 56,566 48.350 50.527 1.00 62.34 HETATM 52 O HOH 52 HETATM 53 O HOH 69.733 31.591 80.417 1.00 84.65 53 HETATM 54 O HOH 54 54.694 40.240 86.738 1.00 70.28 59.333 24.933 73.595 1.00 57.45 HETATM 55 O HOH 55 HETATM 56 O HOH 56 70,409 51,391 81,779 1.00 59,24 HETATM 1 O HOH 57 31.845 31.472 62.530 1.00 29.20 HETATM 2 O HOH 58 32.562 30.513 69.296 1.00 34.69 HETATM 3 O HOH 59 34.498 28.884 70.461 1.00 29.20 HETATM 4 O HOH 60 45,409 26,911 70,363 1,00 32,57 HETATM 5 O HOH 61 34.193 27,990 73.282 1.00 30.58 32.822 24.241 68.673 1.00 40.19 HETATM 6 O HOH 62 HETATM 7 O HOH 33.935 27.969 65.961 1.00 35.49 63

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				1011
HETATM	8 O	HOH	64	30.796 19.159 80.905 1.00 50.10
HETATM	9 O	HOH	65	29.988 26.357 73.687 1.00 40.36
HETATM	10 O	нон	66	46.316 34.186 65.148 1.00 39.13
HETATM	11 0	НОН	67	30.697 30.965 71.805 1.00 50.24
HETATNI	12 O	НОН	68	49.113 27.839 71.457 1.00 47.01
HETATM	13 O	HOH	69	40.944 40.126 48.862 1.00 55.13
HETATM	14 O	НОН	70	32.119 26.221 70.754 1.00 51.01
HETATM	15 O	HOH	71	37.406 41.975 48.996 1.00 47.12
HETATM	16 O	HOH	72	48.657 39.247 50.483 1.00 63.81
HETATM	17 O	HOH	73	26.862 41.181 48.762 1.00 69.42
HETATM	is O	HOH	74	25.401 30.214 67.857 1.00 72.19
HETATM	19 O	НОН	75	30.576 21.546 58.202 1.00 51.83
HETATM	20 O	НОН	76	35.909 14.132 78.132 1.00 62.99
HETATM	21 O	НОН	77	52.634 29.330 63.071 1.00 58.31
HETATM	22 O	HOH	78	26.808 27.051 57.128 1.00 45.94
HETATM	23 O	HOH	79	29.245 28.608 55.705 1.00 83.48
HETATM	24 O	HOH	80	29.129 27.091 76.317 1.00 33.47
HETATNI	25 O	HOH	81	33.625 38.647 81.633 1.00 41.20
HETATN	26 O	HOH	82	36.603 51.147 53.895 1.00 48.15
HETATM	27 O	HOH	83	28.622 46.426 60.451 1.00 52.33
HETATM	28 O	HOH	84	38.056 53.295 65.884 1.00 60.11
HETATM	29 O	HOH	85	43.521 38.970 58.179 1.00 51.73
HETATN	30 O	HOH	86	27.777 37.624 76.264 1.00 70.19
HETATM	31 O	HOH	87	22.739 30.334 60.747 1.00 67.64
HETATM	32 O	HOH	88	26.762 28.420 86.838 1.00 65.95
HETATM	33 O	HOH	89	39.032 29.779 46.494 1.00 89.14
HETATN	34 O	HOH	90	34.718 26.674 68.385 1.00 47.22
HETATM	35 O	HOH	91	29.738 28.093 71.095 1.00 44.84
HETATM	36 O	HOH	92	55.506 30.331 64.286 1.00 70.99
HETATM	37 O	HOH	93	29.692 12.806 76.719 1.00 53.32
HETATNI	38 O	HOH	94	29.342 24.024 63.816 1.00 67.83
HETATM	39 O	HOH		29.596 43.489 50.236 1.00 55.40
HETATNI	40 O	HOH	96	33.505 15.266 63.104 1.00 76.39
HETATM	41 O	HOH	97	36.057 14.492 70.938 1.00 71.41
HETATNI	42 O	HOH	98	26.881 34.813 73.143 1.00 72.62
HETATNI	43 O	HOH	99	27.506 35.250 67.027 1.00 53.58
HETATNI	44 O	HOH	100	25.166 33.321 65.780 1.00 85.60
END				

FIGURE 21

08-SEP-97 1ERE HEADER NUCLEAR RECEPTOR TITLE HUMAN OESTROGEN RECEPTOR LIGAND-BINDING DOMAIN IN COMPLEX TITLE 2 WITH 17BETA-OESTRADIOL COMPND MOL ID: 1; COMPND 2 MOLECULE: OESTROGEN RECEPTOR; COMPND 3 CHAIN: A, B, C, D, E, F; COMPND 4 FRAGMENT: LIGAND-BINDING DOMAIN; COMPND 5 SYNONYM: ESTROGEN RECEPTOR, ER-LBD; COMPND 6 BIOLOGICAL_UNIT: DIMER; COMPND 7 OTHER DETAILS: LIGAND-BINDING DOMAIN COMPND 8 (DOMAIN E - RESIDUES 301-553) IN COMPLEX WITH ENDOGENOUS COMPND 9 LIGAND 17BETA-OESTRADIOL SOURCE MOL ID: 1; SOURCE 2 ORGANISM_SCIENTIFIC: HOMO SAPIENS; SOURCE 3 ORGANISM_COMMON: HUMAN; SOURCE 4 STRAIN: JM109; SOURCE 5 VARIANT: C1857; SOURCE 6 PLASMID: PEALPHA 35; SOURCE 7 GENE: ER ALPHA KEYWDS , NUCLEAR RECEPTOR, TRANSCRIPTION FACTOR, STEROID, AGONIST AUTHOR A.M.BRZOZOWSKI, A.C.W.PIKE REMARK 1 REMARK 2 REMARK 2 RESOLUTION. 3.1 ANGSTROMS. REMARK 3 REMARK 3 REFINEMENT. REMARK 3 PROGRAM : REFMAC REMARK 3 AUTHORS : MURSHUDOV, VAGIN, DODSON REMARK 3 REMARK 3 DATA USED IN REFINEMENT. REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS): 3.1 REMARK 3 RESOLUTION RANGE LOW (ANGSTROMS): 20 (SIGMA(F)): 0 REMARK 3 DATA CUTOFF REMARK 3 COMPLETENESS FOR RANGE (%): 99.1 REMARK 3 NUMBER OF REFLECTIONS : 33981 REMARK 3 REMARK 3 FIT TO DATA USED IN REFINEMENT. REMARK 3 CROSS-VALIDATION METHOD : THROUGHOUT REMARK 3 FREE R VALUE TEST SET SELECTION: RANDOM REMARK 3 R VALUE (WORKING + TEST SET): NONE REMARK 3 R VALUE (WORKING SET): 0.218 REMARK 3 FREE R VALUE : 0.251

REMARK 3 FREE R VALUE TEST SET SIZE (%): 10

REMARK 3 FREE R VALUE TEST SET COUNT : 3398

REMARK 3

REMARK 6 ER-LBD WAS CARBOXYMETHYLATED PRIOR TO CRYSTALLISATION

BUT

REMARK 5 MODIFIED CYSTEINES ARE NOT MODELLED IN THIS ENTRY.

REMARK 7

REMARK 7 RESIDUES LEU306, LEU466, LEU469, LYS492, LYS531 AND LEU536

REMARK 7 (CHAINS ABCDEF) WERE POORLY RESOLVED IN THE ELECTRON

REMARK 7 DENSITY MAPS AND ARE NOT FULLY MODELLED IN THIS ENTRY.

REMARK S

REMARK S RESIDUES MODELLED IN ALTERNATE CONFORMATIONS (CHAINS

REMARK 8 ABCDEF): 377,501,513,530

REMARK 399

REMARK 999 SEQUENCE

REMARK 999 REFERENCE: REFERENCE: SER A 301 - ASN A 304 MISSING FROM

REMARK 999 PDB DUE TO DISORDER TYR A 331 - PRO A 336 MISSING FROM

REMARK 999 PDB DUE TO DISORDER LEU A 462 - SER A 464 MISSING FROM

REMARK 999 PDB DUE TO DISORDER LEU A 549 - THR A 553 MISSING FROM

REMARK 999 PDB DUE TO DISORDER.

REMARK 999 REFERENCE: REFERENCE: SER B 301 - ASN B 304 MISSING FROM

REMARK 999 PDB DUE TO DISORDER TYR B 331 - PRO B 336 MISSING FROM

REMARK 999 PDB DUE TO DISORDER LEU B 462 - SER B 464 MISSING FROM

REMARK 999 PDB DUE TO DISORDER LEU B 549 - THR B 553 MISSING FROM

REMARK 999 PDB DUE TO DISORDER.

REMARK 999 REFERENCE: REFERENCE: SER C 301 - ASN C 304 MISSING FROM

REMARK 999 PDB DUE TO DISORDER TYR C 331 - PRO C 336 MISSING FROM

REMARK 999 PDB DUE TO DISORDER LEU C 462 - SER C 464 MISSING FROM

REMARK 999 PDB DUE TO DISORDER LEU C 549 - THR C 553 MISSING FROM

REMARK 999 PDB DUE TO DISORDER. REMARK 999 REFERENCE: REFERENCE: SER D 301 - ASN D 304 MISSING FROM REMARK 999 PDB DUE TO DISORDER TYR D 331 - PRO D 336 MISSING FROM REMARK 999 PDB DUE TO DISORDER LEU D 462 - SER D 464 MISSING FROM REMARK 999 PDB DUE TO DISORDER LEU D 549 - THR D 553 MISSING FROM REMARK 999 PDB DUE TO DISORDER. REMARK 999 REFERENCE: REFERENCE: SER E 301 - ASN E 304 MISSING FROM REMARK 999 PDB DUE TO DISORDER TYR E 331 - PRO E 336 MISSING FROM REMARK 999 PDB DUE TO DISORDER LEU E 462 - SER E 464 MISSING FROM REMARK 999 PDB DUE TO DISORDER LEU E 549 - THR E 553 MISSING FROM REMARK 999 PDB DUE TO DISORDER. REMARK 999 REFERENCE: REFERENCE: SER F 301 - ASN F 304 MISSING FROM REMARK 999 PDB DUE TO DISORDER TYR F 331 - PRO F 336 MISSING FROM REMARK 999 PDB DUE TO DISORDER LEU F 462 - SER F 464 MISSING FROM REMARK 999 PDB DUE TO DISORDER LEU F 549 - THR F 553 MISSING FROM REMARK 999 PDB DUE TO DISORDER. CRYST1 61.480 115.160 137.380 90.00 98.80 90.00 P 1 21 1 12 ORIGX1 1.000000 0.000000 0.000000 0.00000 0.000000 1.000000 0.000000 ORIGX2 0.00000 ORIGX3 0.000000 0.000000 1.000000 0.00000 0.016265 0.000000 0.002518 SCALE1 0.00000 SCALE2 0.000000 0.008684 0.000000 0.00000 0.000000 0.000000 0.007366 SCALE3 0.00000

N ATOM 1 N SER A 305 22.376 70.539 109.257 1.00 90.58 21.381 69.729 110.019 1.00 89.92 ATOM 2 CA SER A 305 С ATOM 3 C SER A 305 20.264 70.593 110.587 1.00 89.41 C 0 ATOM 4 O SER A 305 20.539 71.556 111.320 1.00 89.09 22.072 68.944 111.149 1.00 89.79 ATOM 5 CB SER A 305 C 0 ATOM 6 OG SER A 305 21.136 68.215 111.938 1.00 89.19 7 N LEU A 306 19.015 70.206 110.299 1.00 88.77 N ATOM 8 CA LEU A 306 17.865 70.930 110.863 1.00 88.07 C ATOM 9 C LEU A 306 18.131 71.087 112.365 1.00 86.68 C ATOM 0 ATOM 10 O LEU A 306 18.154 72.187 112.907 1.00 86.51

C 16.542 70.192 110.645 1.00 88.32 11 CB LEU A 306 ATOM N 18,397 69,974 113,039 1,00 84.80 15 N ALA A 307 **ATOM** 18.729 69.938 114.436 1.00 83.76 C 16 CA ALA A 307 **ATOM** C 19.481 71.204 114.826 1.00 83.39 17 C ALA A 307 **ATOM** 0 18 O ALA A 307 18.990 71.996 115.641 1.00 83.52 **ATOM** C 19.658 68.756 114.709 1.00 84.44 19 CB ALA A 307 **ATOM** 20.651 71.396 114.216 1.00 82.63 N 20 N LEU A 308 **ATOM** 21,450 72,573 114,519 1.00 82.87 C 21 CA LEU A 308 **ATOM** C 20.880 73.922 114.137 1.00 83.17 22 C LEU A 308 **ATOM** 21,524 74,938 114,470 1.00 85.07 0 23 O LEUA 308 **ATOM** 22.856 72.405 113.918 1.00 82.50 C 24 CB LEU A 308 **ATOM** C 23.622 71.169 114.406 1.00 82.65 **ATOM** 25 CG LEU A 308 25.115 71.374 114.134 1.00 82.32 C 26 CD1 LEU A 308 **ATOM** 23,409 70,923 115,910 1.00 82,67 C 27 CD2 LEU A 308 **ATOM** 19.730 74.056 113.506 1.00 82.11 N 28 N SER A 309 **ATOM** 19.152 75.332 113.145 1.00 81.35 C 29 CA SER A 309 ATOM 17.899 75.697 113.915 1.00 79.81 C ATOM 30 C SER A 309 17.635 76.897 114.084 1.00 80.42 O **ATOM** 31 O SER A 309 18.766 75.242 111.654 1.00 83.07 C 32 CB SER A 309 ATOM 0 19.898 74.642 110.994 1.00 85.37 **ATOM** 33 OG SER A 309 17.120 74.699 114.355 1.00 77.25 N 34 N LEU A 310 ATOM 15.904 75.058 115.082 1.00 74.54 C **ATOM** 35 CA LEU A 310 16.256 75.861 116.330 1.00 73.69 C 36 C LEU A 310 ATOM 17.351 75.858 116.884 1.00 73.90 0 37 O LEU A 310 ATOM 15.045 73.869 115.438 1.00 74.07 C 38 CB LEU A 310 **ATOM** 15.143 72.689 114.475 1.00 74.30 C 39 CG LEU A 310 **ATOM** 15.798 71.520 115.196 1.00 74.63 C 40 CD1 LEU A 310 **ATOM** 13.775 72.311 113.936 1.00 74.41 C 41 CD2 LEU A 310 ATOM 15.256 76.611 116.750 1.00 72.43 N 42 N THR A 311 **ATOM** C 15.398 77.463 117.933 1.00 71.67 43 CA THR A 311 ATOM 14.918 76.624 119.094 1.00 70.84 C 44 C THR A 311 ATOM O 14.145 75.689 118.807 1.00 70.32 45 O THR A 311 **ATOM** C 46 CB THR A 311 14.566 78.734 117.727 1.00 72.13 ATOM 0 13.163 78.469 117.614 1.00 71.92 47 OG1 THR A 311 ATOM C 14,993 79,395 116,418 1.00 72,78 48 CG2 THR A 311 ATOM N 15.271 76.947 120.334 1.00 70.12 49 N ALA A 312 **ATOM** C 14.791 76.149 121.458 1.00 69.91 50 CA ALA A 312 ATOM C 13.291 75.914 121.324 1.00 70.10 51 C ALA A 312 **ATOM** O 12.840 74.799 121.594 1.00 70.35 52 O ALA A 312 ATOM C 53 CB ALA A 312 15.085 76.752 122.801 1.00 69.80 **ATOM** N 12.549 76.922 120.901 1.00.70.79 54 N ASP A 313 **ATOM** C 55 CA ASP A 313 11.123 76.716 120.726 1.00 72.57 **ATOM** C 56 C ASP A 313 10.756 75.706 119.664 1.00 70.70 ATOM 57 O ASP A 313 9.870 74.885 119.911 1.00 69.68 0 ATOM C 10.481 78.090 120.476 1.00 76.96 58 CB ASP A 313 **ATOM**

13.114 67.526 122.055 1.00 50.58

C

ATOM

103 CD1 LEU A 319

113/371

		- 1	
ATOM	104 CD2 LEU A 319	12.767 65.812 120.232 1.00 50.24	C
ATOM	105 N LEU A 320	7.794 67.582 120.885 1.00 56.70	N
ATOM	106 CA LEU A 320	6.426 67.386 121.372 1.00 58.80	С
ATOM	107 C LEU A 320	5.587 66.689 120.321 1.00 61.20	С
ATOM	108 O LEU A 320	4.718 65.871 120.579 1.00 61.72	Ο
ATOM	109 CB LEU A 320	5.867 68.750 121.783 1.00 57.70	С
ATOM	110 CG LEU A 320	6.105 68.990 123.269 1.00 57.68	С
ATOM	111 CD1 LEU A 320	5.658 70.368 123.692 1.00 58.75	. C
ATOM	112 CD2 LEU A 320	5.402 67.915 124.081 1.00 57.28	C
ATOM	113 N ASP A 321	5.845 67.007 119.060 1.00 64.39	N
ATOM	114 CA ASP A 321	5.155 66.399 117.958 1.00 67.83	С
ATOM	115 C ASP A 321	5.484 64.951 117.672 1.00 66.45	С
ATOM		4.575 64.205 117.304 1.00 68.09	Ο
ATOM		5.561 67.162 116.682 1.00 73.23	С
ATOM		4.371 68.049 116.346 1.00 78.17	C
ATOM	119 OD1 ASP A 321		0
ATOM	120 OD2 ASP A 321	4.437 68.658 115.254 1.00 81.45	0
ATOM	121 N ALA A 322	6.742 64.551 117.828 1.00 62.92	N
ATOM		7.106 63.176 117.533 1.00 59.78	С
ATOM	123 C ALA A 322		С
ATOM	124 O ALA A 322	6,491 60,986 118,187 1,00 58,35	Ο
ATOM	125 CB ALA A 322	8.623 63.125 117.574 1.00 59.62	С
ATOM	126 N GLU A 323	6.006 62.621 119.645 1.00 56.77	N
ATOM	127 CA GLU A 323	5.470 61.696 120.623 1.00 55.49	C
ATOM	128 C GLU A 323	4.598 60.657 119.989 1.00 55.69	C
ATOM	129 O GLU A 323	3.777 60.975 119.138 1.00 58.08	Ο
ATOM	130 CB GLU A 323	4.775 62.515 121.690 1.00 55.82	С
ATOM	131 CG GLU A 323	5.822 63.073 122.666 1.00 57.00	С
ATOM	132 CD GLU A 323	6.302 61.945 123.557 1.00 57.18	С
ATOM	133 OE1 GLU A 323	5.500 61.285 124.241 1.00 57.59	О
ATOM	134 OE2 GLU A 323	7.506 61.678 123.584 1.00 57.83	O
ATOM	135 N PRO A 324	4.769 59.403 120.344 1.00 55.05	N.
ATOM	136 CA PRO A 324	3.992 58.282 119.878 1.00 54.38	С
ATOM	137 C PRO A 324	2.646 58.236 120.586 1.00 54.98	С
ATOM	138 O PRO A 324	2.391 58.938 121.554 1.00 55.02	О
ATOM	139 CB PRO A 324	4.750 57.015 120.307 1.00 54.50	С
ATOM	140 CG PRO A 324	5.488 57.513 121.513 1.00 54.68	С
ATOM	141 CD PRO A 324	5.735 58.996 121.376 1.00 55.35	С
ATOM	142 N PRO A 325	1.758 57.400 120.099 1.00 56.07	N
ATOM	143 CA PRO A 325	0.428 57.188 120.623 1.00 56.86	С
ATOM	144 C PRO A 325	0.524 56.397 121.916 1.00 57.84	C
ATOM	145 O PRO A 325	1.583 55.785 122.033 1.00 58.89	0
ATOM	146 CB PRO A 325	-0.290 56.266 119.622 1.00 57.07	С
ATOM	147 CG PRO A 325	0.861 55.568 118.950 1.00 56.52	C
ATOM	148 CD PRO A 325	2.021 56.531 118.938 1.00 56.97	С

193 CA PHE A 337

-1.980 37.049 136.956 1.00 85.09

C

ATOM

wo	98/56812	116/371	PCT/GB98/01708
ATOM	239 C MET A 343	4.863 38.836 130.511 1.00 57.16	C
ATOM		5.226 39.762 129.786 1.00 58.46	0
ATOM	241 CB MET A 343	6.431 37.550 131.961 1.00 56.18	C
ATOM	242 CG MET A 343	7.321 37.682 133.190 1.00 56.31	C
ATOM	243 SD MET A 343	8.204 39.248 133.273 1.00 56.60	S
ATOM		8.874 39.359 131.604 1.00 55.24	C
ATOM		3.925 37.967 130.120 1.00 55.99	N
ATOM		3.273 38.073 128.833 1.00 53.83	C
ATOM	247 C GLY A 344	2.718 39.465 128.578 1.00 52.90	C
ATOM		3.122 40.066 127.583 1.00 53.02 1.827 40.019 129.394 1.00 52.76	O N
ATOM		1.305 41.347 129.094 1.00 53.20	C
ATOM	250 CA LEU A 345	2.394 42.408 128.910 1.00 52.33	c
ATOM	251 C LEU A 343	2.487 43.119 127.925 1.00 52.10	O
ATOM	252 O LEU A 345	0.464 41.917 130.219 1.00 54.25	C
ATOM		-0.848 41.244 130.534 1.00 55.33	Č
ATOM		-0.756 40.738 131.968 1.00 56.61	C
ATOM		-1.953 42.272 130.348 1.00 55.75	Č
ATOM	257 N LEU A 346		N
ATOM		4.281 43.498 130.014 1.00 48.34	C
ATOM		5.124 43.395 128.760 1.00 47.59	С
ATOM	260 O LEU A 346	5.370 44.335 128.000 1.00 47.20	0
ATOM	261 CB LEU A 346	5.013 43.231 131.323 1.00 47.25 4.269 43.696 132.570 1.00 46.58 5.252 43.653 133.732 1.00 46.95	. C
ATOM	262 CG LEU A 346	4.269 43.696 132.570 1.00 46.58	C .
ATOM	263 CD1 LEU A 346	5.252 43.653 133.732 1.00 46.95	C
ATOM	264 CD2 LEU A 346	3.689 45.090 132.428 1.00 45.64	С
ATOM		5.556 42.174 128.487 1.00 46.40	N
ATOM		6.374 41.860 127.321 1.00 45.75	С
ATOM		5.697 42.169 126.020 1.00 46.81	C
ATOM		6.265 42.727 125.081 1.00 46.83	0
ATOM	•	6.733 40.397 127.565 1.00 45.43	C
ATOM	270 OG1 THR A 347	8.148 40.411 127.801 1.00 47.31	0
ATOM	271 CG2 THR A 347	6.253 39.444 126.535 1.00 44.20	C N
ATOM	272 N ASN A 348	4.409 41.866 125.902 1.00 48.83 3.607 42.153 124.716 1.00 48.72	C
ATOM	273 CA ASN A 348 274 C ASN A 348	3.511 43.662 124.507 1.00 47.34	C
ATOM ATOM	274 C ASN A 348 275 O ASN A 348	3.719 44.247 123.449 1.00 47.88	O
ATOM	276 CB ASN A 348	2.210 41.560 124.918 1.00 51.06	C
ATOM	277 CG ASN A 348	1.272 41.891 123.765 1.00 54.34	Č
ATOM	278 OD1 ASN A 348	0.504 42.881 123.743 1.00 55.31	O
ATOM	279 ND2 ASN A 348	1.371 40.995 122.770 1.00 55.16	N
ATOM	280 N LEU A 349	3.194 44.396 125.563 1.00 45.51	N
ATOM	281 CA LEU A 349	3.045 45.841 125.500 1.00 43.88	C
ATOM	282 C LEU A 349	4.366 46.413 125.034 1.00 44.02	C
ATOM	283 O LEU A 349	4.397 47.250 124.128 1.00 43.98	O

wo	98/56812	117/371	PCT/GB98/01708
АТОМ	284 CB LEU A 349	2.597 46.340 126.878 1.00 44.61	С
ATOM	285 CG LEU A 349		C .
	286 CD1 LEU A 349	1.354 48.294 125.964 1.00 45.55	С
		2.014 48.325 128.358 1.00 45.19	С
ATOM	288 N ALA A 350	5.489 45.958 125.615 1.00 43.72	N
ATOM		6.818 46.432 125.216 1.00 42.64	С
ATOM		7.023 46.190 123.724 1.00 42.80	С
ATOM		7.291 47.135 122.996 1.00 42.61	0
ATOM		7.949 45.739 125.956 1.00 41.26	С
ATOM		6.839 44.944 123.276 1.00 43.48	N
ATOM		6.997 44.638 121.871 1.00 45.42	· C
		6.223 45.576 120.945 1.00 45.86	C
		6.686 45.967 119.856 1.00 46.01	0
		6.633 43.184 121.612 1.00 47.72	C
ATOM	298 CG ASP A 351	6.905 42.840 120.149 1.00 50.33	C
ATOM	299 OD1 ASP A 351	8.043 42.706 119.656 1.00 49.95 5.887 42.687 119.433 1.00 53.18	0
	300 OD2 ASP A 351	5.887 42.687 119.433 1.00 53.18	0
ATOM		5.018 45.967 121.331 1.00 45.40	N C
		4.237 46.886 120.529 1.00 45.67 4.783 48.299 120.572 1.00 46.20	C
ATOM	303 C ARG A 352	4.783 48.299 120.372 1.00 46.20	0
ATOM			C
ATOM ATOM		2.817 46.836 121.056 1.00 46.38 2.174 45.538 120.584 1.00 48.04	C
		0.680 45.902 120.387 1.00 50.42	
		0.095 45.703 121.723 1.00 52.44	
		-0.723 46.610 122.289 1.00 53.34	
ATOM	310 NH1 ARG A 352	-1.042 47.739 121.644 1.00 52.42	N
		-1.132 46.217 123.500 1.00 53.07	
		5.141 48.837 121.745 1.00 45.01	N
		5.680 50.194 121.773 1.00 43.53	С
		6.968 50.299 120.966 1.00 42.80	
ATOM	315 O GLU A 353	7.305 51.370 120.459 1.00 43.00	0
ATOM	316 CB GLU A 353	5.966 50.620 123.198 1.00 43.41	C
ATOM	317 CG GLU A 353	4.910 50.245 124.204 1.00 44.09	C ·
ATOM	318 CD GLU A 353	5.154 50.924 125.538 1.00 44.78	С
ATOM	319 OE1 GLU A 353	5.187 52.154 125.617 1.00 43.92	0
ATOM	320 OE2 GLU A 353	5.323 50.176 126.525 1.00 46.56	0
ATOM	321 N LEU A 354	7.704 49.198 120.834 1.00 41.84	N
ATOM	322 CA LEU A 354	8.969 49.195 120.124 1.00 42.17	С
ATOM	323 C LEU A 354	8.804 49.655 118.698 1.00 42.86	C .
ATOM	324 O LEU A 354	9.616 50.399 118.160 1.00 42.54	0
ATOM	325 CB LEU A 354	9.642 47.827 120.218 1.00 41.39	C
ATOM	326 CG LEU A 354	10.467 47.775 121.518 1.00 41.35	C
ATOM	327 CD1 LEU A 354	10.648 46.351 121.978 1.00 41.91	C
ATOM	328 CD2 LEU A 354	11.783 48.483 121.295 1.00 41.15	C

wo	98/56812	118/371	PCT/GB98/01708
ATOM	329 N VAL A 355	7.698 49.203 118.103 1.00 43.57	N
ATOM	330 CA VAL A 355	7.424 49.649 116.733 1.00 42.80	C
ATOM	331 C VAL A 355	7.268 51.167 116.754 1.00 44.35	C
ATOM	332 O VAL A 333	7.982 51.901 116.058 1.00 44.80	O C
ATOM	333 CD AME W 333	6.142 48.974 116.268 1.00 40.41 5.838 49.431 114.878 1.00 39.85	C
ATOM ATOM		6.385 47.492 116.364 1.00 41.41	C
ATOM		6.361 51.672 117.597 1.00 44.18	N
ATOM		6.178 53.115 117.631 1.00 45.93	C
ATOM	338 C HIS A 356	7.484 53.818 117.909 1.00 44.50	c
ATOM	339 O HIS A 356	7.691 54.886 117.348 1.00 44.30	Ö
ATOM		5.074 53.470 118.667 1.00 49.34	C
ATOM	341 CG HIS A 356	3.801 52.906 118.115 1.00 51.75	Č
ATOM	342 ND1 HIS A 356	2.806 53.687 117.571 1.00 53.41	N
ATOM	343 CD2 HIS A 356	3.801 52.906 118.115 1.00 51.75 2.806 53.687 117.571 1.00 53.41 3.422 51.617 117.985 1.00 52.93	C
ATOM	344 CE1 HIS A 356	1.840 52.884 117.133 1.00 54.25	С
ATOM	345 NE2 HIS A 356	2.186 51.619 117.369 1.00 54.33	N
ATOM	346 N MET A 357	8.303 53.240 118.784 1.00 43.74	N
ATOM		9.564 53.819 119.185 1.00 43.00	С
ATOM		10.472 54.177 118.015 1.00 42.86	C
ATOM		10.973 55.288 117.903 1.00 42.82	0
ATOM		10.385 52.909 120.117 1.00 42.65	C
ATOM	351 CG MET A 357	11.501 53.799 120.720 1.00 43.39	C
ATOM	352 SD MET A 357	12.579 52.768 121.725 1.00 44.21	S . C
		11.526 52.625 123.168 1.00 44.48	N
ATOM ATOM		10.665 53.188 117.151 1.00 42.08 11.465 53.306 115.961 1.00 40.73	C
ATOM		10.980 54.507 115.168 1.00 42.35	c
ATOM		11.811 55.315 114.760 1.00 43.21	O
ATOM		11.334 52.029 115.114 1.00 39.01	C
ATOM		11.888 50.851 115.908 1.00 38.76	C
ATOM	360 CG2 ILE A 358	12.064 52.170 113.799 1.00 37.79	Ċ
ATOM	361 CD1 ILE A 358	11.865 49.519 115.206 1.00 38.39	С
ATOM	362 N ASN A 359	9.683 54.631 114.950 1.00 44.26	N
ATOM	363 CA ASN A 359	9.114 55.742 114.220 1.00 46.79	С
ATOM	364 C ASN A 359	9.443 57.060 114.880 1.00 46.25	С
ATOM	365 O ASN A 359	9.899 58.021 114.275 1.00 48.11	0
ATOM	366 CB ASN A 359	7.587 55.634 114.159 1.00 51.74	C
ATOM	367 CG ASN A 359	7.290 54.604 113.091 1.00 56.17	С
ATOM	368 OD1 ASN A 359	7.650 54.927 111.954 1.00 60.30	0
ATOM	369 ND2 ASN A 359	6.727 53.450 113.387 1.00 57.83	N
ATOM	370 N TRP A 360	9.230 57.118 116.178 1.00 44.87	N
ATOM	371 CA TRP A 360		C C
ATOM	372 C TRP A 360	10.969 58.707 116.765 1.00 43.83	0
ATOM	373 O TRP A 360	11.335 59.846 116.544 1.00 44.37	

		((()) ()	
ATOM	374 CB TRP A 360	9.268 57.954 118.392 1.00 42.53	С
ATOM	375 CG TRP A 360	9.913 58.953 119.301 1.00 43.10	С
ATOM	376 CD1 TRP A 360	9.463 60.210 119.571 1.00 43.10	С
ATOM	377 CD2 TRP A 360	11.114 58.770 120.057 1.00 43.07	С
ATOM	378 NE1 TRP A 360	10.314 60.817 120.448 1.00 43.67	N
ATOM	379 CE2 TRP A 360	11.335 59.958 120.768 1.00 43.61	С
ATOM	380 CE3 TRP A 360	12.019 57.723 120.194 1.00 43.09	С
ATOM	381 CZ2 TRP A 360	12.426 60.150 121.617 1.00 43.58	С
ATOM	382 CZ3 TRP A 360	13.102 57.920 121.024 1.00 44.07	С
ATOM	383 CH2 TRP A 360	13.304 59.111 121.732 1.00 43.80	С
ATOM	384 N ALA A 361	11.869 57.735 116.888 1.00 45.32	N
ATOM	385 CA ALA A 361	13.303 57.983 116.771 1.00 45.58	С
ATOM	386 C ALA A 361	13.575 58.748 115.489 1.00 46.83	С
ATOM	387 O ALA A 361	14.330 59.719 115.538 1.00 46.98	Ο
ATOM	388 CB ALA A 361	14.078 56.686 116.840 1.00 44.50	С
ATOM	389 N LYS A 362	12.959 58.380 114.372 1.00 48.34	N
ATOM	390 CA LYS A 362	13.207 59.033 113.106 1.00 50.58	С
ATOM	391 C LYS A 362	12.907 60.508 113.100 1.00 50.88	С
ATOM	392 O LYS A 362	13.456 61.175 112.231 1.00 51.42	О
ATOM		12.485 58.322 111.966 1.00 52.62	С
ATOM	394 CG LYS A 362	13.035 56.917 111.760 1.00 55.71	С
ATOM	395 CD LYS A 362		С
ATOM	396 CE LYS A 362		С
ATOM		15.709 56.341 109.035 1.00 64.54	N
ATOM	398 N ARG A 363		N
ATOM		11.785 62.450 114.045 1.00 53.69	С
ATOM	400 C ARG A 363		С
ATOM	401 O ARG A 363		0_
ATOM		10.315 62.631 114.474 1.00 56.98	C
ATOM		9.582 61.312 114.322 1.00 63.56	C
ATOM	404 CD ARG A 363		С
ATOM	405 NE ARG A 363		N
ATOM	406 CZ ARG A 363	6.929 62.184 113.480 1.00 78.35	C
ATOM	407 NH1 ARG A 363	6.676 61.046 114.134 1.00 79.67	N
ATOM	408 NH2 ARG A 363	6.051 63.193 113.446 1.00 80.13	N
ATOM	409 N VAL A 364	13.507 62.599 115.836 1.00 51.20	N
ATOM	410 CA VAL A 364	14.219 63.406 116.858 1.00 48.91	С
ATOM	411 C VAL A 364	15.256 64.176 116.076 1.00 48.54	C
ATOM	412 O VAL A 364	16.138 63.589 115.462 1.00 49.24	0
ATOM	413 CB VAL A 364	14.821 62.482 117.916 1.00 47.40	c
ATOM	414 CG1 VAL A 364	15.741 63.200 118.872 1.00 46.24	C
ATOM	415 CG2 VAL A 364	13.677 61.813 118.654 1.00 47.03	C
ATOM	416 N PRO A 365	15.170 65.480 116.033 1.00 48.39	N
ATOM	417 CA PRO A 365	16.097 66.322 115.282 1.00 47.91	C
ATOM	418 C PRO A 365	17.509 65.821 115.405 1.00 47.69	С

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ATOM	419 O PRO A 365	17.971 65.570 116.509 1.00 49.38	O
ATOM		15.903 67.748 115.822 1.00 47.32	С
ATOM		14.412 67.652 116.118 1.00 48.06	С
ATOM	422 CD PRO A 365		С
ATOM	423 N GLY A 366		N
ATOM	424 CA GLY A 366	19.573 65.178 114.242 1.00 47.06	С
ATOM	425 C GLY A 366	19.776 63.692 114.099 1.00 47.16	С
ATOM	426 O GLY A 366	20.835 63.259 113.659 1.00 47.88	О
ATOM	427 N PHE A 367	18.790 62.889 114.477 1.00 47.22	N
ATOM		18.889 61.440 114.464 1.00 47.22	С
ATOM	429 C PHE A 367		C
ATOM	430 () PHE A 367		0
ATOM		17.594 60.806 114.968 1.00 46.00	C
ATOM		17.697 59.321 115.172 1.00 46.50	C
ATOM		18.426 58.795 116.232 1.00 46.47	C C
ATOM		17.067 58.441 114.309 1.00 46.08	C
ATOM		18.523 57.432 116.438 1.00 46.01 17.160 57.074 114.528 1.00 46.50	C
ATOM	436 CE2 PHE A 367		c
ATOM	438 N VAL A 368		N
ATOM ATOM		18.374 60.858 110.797 1.00 47.41	Ċ
ATOM	440 C VAL A 368		c
ATOM		19.901 60.612 109.101 1.00 48.36	ő
ATOM		17.125 61.454 110.136 1.00 46.86	C.
ATOM	443 CG1 VAL A 368	17,420 62.152 108.846 1.00 47.96	С
ATOM	444 CG2 VAL A 368	16.101 60.354 109.960 1.00 46.89	С
ATOM	445 N ASP A 369	20.424 62.189 110.616 1.00 48.68	N
ATOM	446 CA ASP A 369	21.695 62.531 110.013 1.00 49.52	С
ATOM	447 C ASP A 369		С
ATOM		23.787 61.548 109.748 1.00 49.03	О
ATOM		22.277 63.845 110.556 1.00 53.35	C
ATOM			C
ATOM	451 OD1 ASP A 369	20.601 65.118 109.393 1.00 59.66	0
ATOM	452 OD2 ASP A 369	21.303 65.885 111.327 1.00 59.04	0
ATOM	453 N LEU A 370	22.522 60.450 111.138 1.00 46.30	N
ATOM	454 CA LEU A 370	23.536 59.428 111.403 1.00 45.24	C
ATOM	455 C LEU A 370	23.457 58.314 110.382 1.00 44.34	С
ATOM	456 O LEU A 370	22.434 58.171 109.701 1.00 43.23 23.300 58.888 112.819 1.00 45.60	O C
ATOM	457 CB LEU A 370	23.446 59.923 113.939 1.00 45.74	C
ATOM	458 CG LEU A 370 459 CD1 LEU A 370	23.173 59.313 115.301 1.00 45.87	C
ATOM ATOM	460 CD2 LEU A 370	24.871 60.487 113.901 1.00 45.51	c
ATOM	461 N THR A 371	24.499 57.499 110.215 1.00 44.24	N
ATOM	462 CA THR A 371	24.364 56.429 109.204 1.00 43.33	Ĉ
ATOM	463 C THR A 371	23.278 55.478 109.682 1.00 44.46	c
AT OM	OJ C TIMAJII	25.270 55.770 107.002 1.00 77.10	-

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ATOM	464 O THR A 371	23.058 55.270 110.884 1.00 44.89	О
ATOM	465 CB THR A 371	25.644 55.614 109.113 1.00 42.88	С
ATOM	466 OG1 THR A 371	25.991 55.295 110.475 1.00 44.81	0
ATOM	467 CG2 THR A 371	26.725 56.466 108.523 1.00 43.53	С
ATOM	468 N LEU A 372	22.612 54.833 108.732 1.00 44.94	N
ATOM	469 CA LEU A 372	21.566 53.878 109.072 1.00 44.26	С
ATOM	470 C LEU A 372		С
ATOM	471 O LEU A 372	21.196 52.643 111.048 1.00 47.02	0
ATOM		21.134 53.178 107.795 1.00 42.97	C
ATOM		20.398 54.060 106.787 1.00 41.97	C
ATOM		20.048 53.301 105.517 1.00 42.70	C
ATOM	475 CD2 LEU A 372	19.081 54.519 107.349 1.00 42.33	С
ATOM	476 N HIS A 373	23.218 52.342 110.147 1.00 46.19	N
ATOM		23.573 51.402 111.202 1.00 46.22	C
ATOM	478 C HIS A 373	23.685 52.125 112.517 1.00 45.75	C
ATOM		23.243 51.528 113.511 1.00 44.61	0
ATOM		24.830 50.649 110.770 1.00 49.78	C
ATOM	481 CG HIS A 373	24.489 49.599 109.749 1.00 52.88	C
ATOM	482 ND1 HIS A 373	24.700 49.707 108.383 1.00 53.25	N
ATOM		23.924 48.383 109.900 1.00 53.27	C
		24.281 48.599 107.798 1.00 53.55	C
		23.789 47.764 108.710 1.00 53.71	N
ATOM	486 N ASP A 374		N C
ATOM		24.295 54.063 113.820 1.00 45.24	
ATOM	488 C ASP A 374		C 0
ATOM	489 O ASP A 374		C
ATOM		25.127 55.336 113.680 1.00 46.38 26.554 54.825 113.562 1.00 49.02	C
ATOM		26.732 53.613 113.888 1.00 49.79	o
ATOM	492 OD1 ASF A 374	27.470 55.582 113.162 1.00 51.05	Ö
ATOM		21.917 54.575 113.648 1.00 42.92	N
ATOM ATOM	495 CA GLN A 375	20.588 54.739 114.188 1.00 42.51	C
ATOM	496 C GLN A 375	20.207 53.417 114.817 1.00 43.01	c
ATOM	497 O GLN A 375	19.822 53.394 115.992 1.00 44.65	Ō
ATOM	498 CB GLN A 375	19.654 55.118 113.076 1.00 43.53	C
ATOM	499 CG GLN A 375	20.088 56.418 112.420 1.00 45.48	С
ATOM	500 CD GLN A 375	19.210 56.773 111.235 1.00 46.42	С
ATOM	501 OE1 GLN A 375	18.039 56.404 111.105 1.00 46.13	0
ATOM	502 NE2 GLN A 375	19.821 57.519 110.324 1.00 47.37	N
ATOM	503 N VAL A 376	20.329 52.291 114.126 1.00 42.62	N
ATOM	504 CA VAL A 376	19.983 51.018 114.772 1.00 42.53	С
ATOM	505 C VAL A 376	20.786 50.895 116.073 1.00 43.65	С
ATOM	506 O VAL A 376	20.260 50.529 117.143 1.00 44.09	0
ATOM	507 CB VAL A 376	20.187 49.810 113.862 1.00 41.72	С
ATOM	508 CG1 VAL A 376	19.460 48.614 114.409 1.00 41.46	С

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ATOM 543 C GLU A 380

ATOM 547 CD GLU A 380

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544 O GLU A 380

545 CB GLU A 380

546 CG GLU A 380

548 OE1 GLU A 380

549 OE2 GLU A 380

550 N CYS A 381

551 CA CYS A 381

552 C CYS A 381

553 O CYS A 381

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SUBSTITUTE SHEET (RULE 26)

19.959 49.277 121.641 1.00 43.23

19.632 48.655 122.633 1.00 44.35

20.396 48.061 119.531 1.00 41.55

19.871 47.462 118.240 1.00 44.58

21,043 46.808 117.525 1.00 46.88

22.196 47.288 117.699 1.00 49.39

20.901 45.823 116.784 1.00 47.67

20.809 50.288 121.736 1.00 44.61

20.382 51.205 123.988 1.00 44.14

20.441 50.771 125.131 1.00 43.47

21.374 50.643 123.006 1.00 46.93

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		123/371	
ATOM	554 CB CYS A 381	22.630 51.531 122.807 1.00 52.10	C
ATOM	555 SG CYS A 381	24.154 50.637 123.375 1.00 64.30	S
ATOM	556 N ALA A 382		N
	557 CA ALA A 382	18.576 52.724 124.604 1.00 40.77	C
	558 C ALA A 382	17.128 52.295 124.647 1.00 41.16	C
ATOM	559 O ALA A 382	16.307 52.896 125.364 1.00 41.74	0
ATOM		18.551 54.208 124.158 1.00 39.48	C
ATOM	561 N TRP A 383	16.712 51.243 123.952 1.00 40.69	N C
ATOM	562 CA TRP A 383	15.292 50.882 123.935 1.00 39.18	C
ATOM	563 C TRP A 383	14.642 50.806 125.292 1.00 38.59	0
ATOM	564 O TRP A 383	13.687 51.543 125.573 1.00 37.35 15.150 49.646 123.083 1.00 38.87	C
ATOM	566 CG TRP A 383		c
ATOM ATOM		16.809 47.778 123.640 1.00 37.73	C
		14.746 47.501 124.465 1.00 37.97	Č
		16.788 46.590 124.331 1.00 37.21	N
ATOM	570 CE2 TRP A 383	15.537 46.405 124.849 1.00 37.91	C
ATOM	571 CE3 TRP A 383	13.407 47.566 124.859 1.00 38.26	C
		15.018 45.371 125.622 1.00 38.84	С
		12.902 46.537 125.625 1.00 38.87	С
ATOM	574 CH2 TRP A 383	13.700 45.447 126.002 1.00 39.04	С
ATOM	575 N LEU A 384	15.177 49.938 126.160 1.00 38.08	N
ATOM	576 CA LEU A 384	14.611 49.807 127.505 1.00 36.09	С
ATOM	577 C LEU A 384	14.721 51.083 128.318 1.00 35.10	C
ATOM		13.826 51.348 129.112 1.00 34.48	0
ATOM		15.207 48.608 128.203 1.00 34.99	C
ATOM		14.603 48.237 129.546 1.00 35.42	C
ATOM		13.092 48.090 129.521 1.00 35.66	C
		15.192 46.892 129.981 1.00 36.23 15.757 51.891 128.156 1.00 35.48	N
ATOM ATOM		15.848 53.129 128.939 1.00 36.88	C
ATOM		14.644 53.984 128.520 1.00 36.73	c
ATOM			0 .
ATOM	587 CB GLU A 385	17.181 53.836 128.798 1.00 38.31	С
ATOM	588 CG GLU A 385	18.326 53.543 129.749 1.00 38.88	С
ATOM	589 CD GLU A 385	19.606 54.258 129.323 1.00 40.96	С
ATOM	590 OE1 GLU A 385	20.219 53.786 128.322 1.00 40.13	Ο
ATOM	591 OE2 GLU A 385	20.062 55.285 129.931 1.00 42.21	Ο
ATOM	592 N ILE A 386	14.496 54.204 127.200 1.00 36.32	N
ATOM	593 CA ILE A 386	13.369 54.952 126.667 1.00 36.91	С
ATOM	594 C ILE A 386	12.015 54.392 127.175 1.00 37.34	C
ATOM	595 O ILE A 386	11.196 55.155 127.686 1.00 36.16	0 .
	596 CB ILE A 386	13.197 54.938 125.148 1.00 37.89	C
	597 CG1 ILE A 386	14.449 55.123 124.299 1.00 39.71	C
ATOM	598 CG2 ILE A 386	12.193 56.015 124.799 1.00 37.70	С

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ATOM	599 CD1 ILE A 386	15.189 56.418 124.439 1.00 40.45	С
ATOM	600 N LEU A 387	11.763 53.082 127.072 1.00 37.39	N
ATOM	601 CA LEU A 387	10.544 52.515 127.573 1.00 37.91	С
ATOM	602 C LEU A 387	10.387 52.805 129.064 1.00 39.68	С
ATOM	603 O LEU A 387	9.240 53.071 129.463 1.00 41.71	Ο
ATOM	604 CB LEU A 387	10.494 50.992 127.494 1.00 38.33	С
ATOM	605 CG LEU A 387	10.120 50.317 126.176 1.00 38.87	С
ATOM	606 CD1 LEU A 387	10.162 48.800 126.371 1.00 37.89	С
ATOM	607 CD2 LEU A 387	8.789 50.804 125.606 1.00 37.40	С
ATOM	608 N MET A 388	11.476 52.739 129.858 1.00 39.41	N
ATOM	609 CA MET A 388	11.300 52.973 131.289 1.00 38.29	С
ATOM	610 C MET A 388	11.054 54.431 131.585 1.00 38.40	С
ATOM	611 O MET A 388	10.187 54.682 132.426 1.00 37.90	Ο
ATOM	612 CB MET A 388	12.409 52.456 132.178 1.00 38.21	С
ATOM	613 CG MET A 388	12.865 51.030 131.946 1.00 39.18	С
ATOM	614 SD MET A 388	13.843 50.384 133.298 1.00 41.37	S
ATOM	615 CE MET A 388	13.780 48.630 133.153 1.00 40.82	С
ATOM	616 N ILE A 389	11.731 55.378 130.921 1.00 39.23	N
ATOM	617 CA ILE A 389	11.393 56.773 131.338 1.00 40.38	С
ATOM	618 C ILE A 389	9.953 57.105 130.980 1.00 41.61	С
ATOM	619 O ILE A 389	9.260 57.885 131.621 1.00 42.10	О
ATOM	620 CB ILE A 389	12.414 57.774 130.800 1.00 39.04	C
ATOM	621 CG1 ILE A 389	12.194 59.163 131.402 1.00 38.47	С
ATOM	622 CG2 ILE A 389	12.297 57.806 129.290 1.00 38.80	С
ATOM	623 CD1 ILE A 389	13.371 60.102 131.204 1.00 37.35	C
ATOM	624 N GLY A 390	9.417 56.498 129.930 1.00 42.82	N
ATOM	625 CA GLY A 390	8.039 56.715 129.508 1.00 44.08	С
ATOM	626 C GLY A 390	7.109 56.228 130.618 1.00 44.05	С
ATOM	627 O GLY A 390	6.226 56.959 131.077 1.00 44.56	О
ATOM	628 N LEU A 391	7.356 54.992 131.035 1.00 42.62	Ν
ATOM	629 CA LEU A 391	6.511 54.453 132.100 1.00 42.62	С
ATOM	630 C LEU A 391		C
ATOM	631 O LEU A 391	5.509 55.728 133.901 1.00 43.15	0
ATOM	632 CB LEU A 391	7.071 53.088 132.498 1.00 42.08	С
ATOM	633 CG LEU A 391	6.485 52.463 133.747 1.00 42.23	С
ATOM	634 CD1 LEU A 391	4.983 52.285 133.530 1.00 43.26	C
ATOM	635 CD2 LEU A 391	7.126 51.127 134.055 1.00 42.49	С
ATOM	636 N VAL A 392	7.704 55.731 133.759 1.00 43.68	N
ATOM	637 CA VAL A 392	7.917 56.545 134.931 1.00 43.90	С
ATOM	638 C VAL A 392	7.100 57.813 134.814 1.00 44.98	C
ATOM	639 O VAL A 392	6.380 58.241 135.708 1.00 45.64	0
ATOM	640 CB VAL A 392	9.422 56.833 135.146 1.00 42.28	C
ATOM	641 CG1 VAL A 392	9.675 57.920 136.172 1.00 42.44	C
ATOM	642 CG2 VAL A 392	10.088 55.603 135.729 1.00 42.06	С
ATOM	643 N TRP A 393	7.242 58.436 133.664 1.00 46.50	N

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ATOM	644 CA TRP A 393	6.584 59.706 133.374 1.00 48.60	С
ATOM	645 C TRP A 393	5.073 59.618 133.392 1.00 49.25	С
ATOM	646 O TRP A 393	4.442 60.477 133.999 1.00 51.00	Ο
ATOM	647 CB TRP A 393	7.008 60.174 131.992 1.00 48.98	С
ATOM	648 CG TRP A 393	6.086 61.190 131.410 1.00 49.25	С
ATOM	649 CD1 TRP A 393	5.226 61.001 130.378 1.00 49.40	С
ATOM	650 CD2 TRP A 393	5.922 62.542 131.826 1.00 49.62	С
ATOM	651 NE1 TRP A 393	4.555 62.170 130.112 1.00 49.05	N
ATOM	652 CE2 TRP A 393	4.964 63.130 130.982 1.00 48.79	С
ATOM	653 CE3 TRP A 393	6.510 63.321 132.824 1.00 50.99	С
ATOM	654 CZ2 TRP A 393	4.580 64.458 131.090 1.00 48.79	C
ATOM	655 CZ3 TRP A 393	6.109 64.656 132.937 1.00 51.01	С
ATOM	656 CH2 TRP A 393	5.160 65.207 132.070 1.00 49.61	С
ATOM	657 N ARG A 394	4.524 58.609 132.717 1.00 49.10	N
ATOM	658 CA ARG A 394	3.079 58.463 132.729 1.00 48.80	С
ATOM	659 C ARG A 394	2.639 57.914 134.078 1.00 50.57	C
ATOM	660 O ARG A 394	1.430 57.901 134.332 1.00 53.43	0
ATOM	661 CB ARG A 394	2.483 57.616 131.634 1.00 47.23	C
ATOM	662 CG ARG A 394	3.134 56.353 131.161 1.00 46.71	C
ATOM	663 CD ARG A 394	2.386 55.724 129.994 1.00 45.21	C
ATOM	664 NE ARG A 394	2.758 54.304 129.908 1.00 45.92	N
ATOM	665 CZ ARG A 394	3.880 53.877 129.315 1.00 45.48	C
ATOM	666 NH1 ARG A 394	4.639 54.850 128.808 1.00 45.47	N
ATOM	667 NH2 ARG A 394	4.192 52.585 129.253 1.00 43.51	N
ATOM	668 N SER A 395	3,506 57,457 134,959 1.00 51,48	N
ATOM	669 CA SER A 395	3.096 56.916 136.243 1.00 52.31	C
ATOM	670 C SER A 395	3.171 57.963 137.341 1.00 54.06	С
ATOM	671 O SER A 395	2.853 57.650 138.486 1.00 53.58 4.040 55.768 136.634 1.00 51.22	O C
ATOM	672 CB SER A 395		Ö
ATOM	673 OG SER A 395		N
ATOM	674 N MET A 396	3.791 60.223 137.959 1.00 60.16	C
ATOM	675 CA MET A 396	2.654 60.519 138.925 1.00 63.28	c
ATOM	676 C MET A 396 677 O MET A 396	2.823 60.538 140.153 1.00 63.48	Õ
ATOM ATOM	678 CB MET A 396	4.030 61.519 137.188 1.00 59.66	C
ATOM	679 CG MET A 396	5.202 62.300 137.761 1.00 60.46	Č
ATOM	680 SD MET A 396	5.832 63.284 136.390 1.00 63.79	S
ATOM	681 CE MET A 396	5.681 64.939 137.052 1.00 63.38	Č
ATOM	682 N GLU A 397	1.464 60.775 138.386 1.00 66.02	N
ATOM	683 CA GLU A 397	0.324 61.111 139.209 1.00 69.12	C
ATOM	684 C GLU A 397	-0.378 59.904 139.747 1.00 67.67	c
ATOM	685 O GLU A 397	-1.597 59.964 139.945 1.00 68.94	Ö
ATOM	686 CB GLU A 397	-0.737 61.932 138.471 1.00 74.43	C
ATOM	687 CG GLU A 397	-0.192 63.107 137.671 1.00 80.96	C
ATOM	688 CD GLU A 397	0.439 62.557 136.400 1.00 85.44	С

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ATOM	689 OE1 GLU A 397	0.066 61.400 136.046 1.00 87.27	0
ATOM	690 OE2 GLU A 397	1.293 63.251 135.796 1.00 88.68	0
ATOM	691 N HIS A 398	0.215 58.755 139.964 1.00 65.64	N
ATOM	692 CA HIS A 398	-0.448 57.589 140.514 1.00 64.64	С
ATOM	693 C HIS A 398	0.563 57.044 141.525 1.00 63.33	С
ATOM	694 O HIS A 398	1.182 56.010 141.286 1.00 64.30	0
ATOM	695 CB HIS A 398	-0.808 56.503 139.512 1.00 65.95	С
ATOM	696 CG HIS A 398	-1.800 56.931 138.480 1.00 67.89	С
ATOM	697 ND1 HIS A 398	-1.581 58.093 137.754 1.00 68.76	N
ATOM	698 CD2 HIS A 398	-2.970 56.441 138.015 1.00 68.33	С
ATOM	699 CE1 HIS A 398	-2.553 58.322 136.904 1.00 68.97	С
ATOM	700 NE2 HIS A 398	-3.408 57.317 137.047 1.00 69.03	N
ATOM	701 N PRO A 399	0.738 57.788 142.593 1.00 60.98	N
ATOM	702 CA PRO A 399	1.678 57.460 143.639 1.00 60.04	С
ATOM	703 C PRO A 399	1.573 56.008 144.013 1.00 58.72	С
ATOM	704 O PRO A 399	0.479 55.479 144.144 1.00 60.15	О
ATOM	705 CB PRO A 399	1.307 58.333 144.857 1.00 60.42	С
ATOM	706 CG PRO A 399	0.722 59.525 144.140 1.00 60.58	С
ATOM	707 CD PRO A 399	0.029 59.010 142.914 1.00 60.38	C
ATOM	708 N GLY A 400	2.676 55.323 144.127 1.00 57.37	N
ATOM	709 CA GLY A 400	2.658 53.933 144.519 1.00 57.37	С
ATOM	710 C GLY A 400	2.241 52.954 143.467 1.00 56.93	С
ATOM	711 O GLY A 400	2.226 51.744 143.762 1.00 57.91	0
ATOM	712 N LYS A 401	1.931 53.447 142.279 1.00 56.53	N
ATOM	713 CA LYS A 401	1.508 52.589 141.185 1.00 56.36	C
ATOM	714 C LYS A 401	2.264 52.906 139.886 1.00 54.56	C
ATOM	715 O LYS A 401	2.864 53.977 139.700 1.00 53.14	0
ATOM	716 CB LYS A 401	0.041 52.772 140.841 1.00 58.66	C
ATOM	717 CG LYS A 401	-0.982 52.903 141.935 1.00 61.77	C
ATOM	718 CD LYS A 401	-1.890 51.680 141.909 1.00 65.18	C
ATOM	719 CE LYS A 401	-2.620 51.475 143.237 1.00 66.98	C
ATOM	720 NZ LYS A 401	-3.156 52.790 143.712 1.00 69.54	N
ATOM	721 N LEU A 402	2.172 51.896 139.007 1.00 51.98	N
ATOM	722 CA LEU A 402	2.813 52.052 137.708 1.00 50.19	C
ATOM	723 C LEU A 402	1.734 51.837 136.656 1.00 49.79	C
ATOM	724 O LEU A 402	1.148 50.766 136.579 1.00 50.90	0
ATOM	725 CB LEU A 402	3.972 51.108 137.434 1.00 49.03	C
ATOM	726 CG LEU A 402	5.170 51.118 138.369 1.00 48.58	C
ATOM	727 CD1 LEU A 402	5.995 49.842 138.211 1.00 49.67	C
ATOM	728 CD2 LEU A 402	6.035 52.333 138.144 1.00 46.96	C
ATOM	729 N LEU A 403	1.485 52.844 135.859 1.00 48.94	N
ATOM	730 CA LEU A 403	0.560 52.836 134.755 1.00 48.00	C
ATOM	731 C LEU A 403	1.171 52.346 133.445 1.00 48.26	C
ATOM	732 O LEU A 403	1.502 53.141 132.540 1.00 46.38	0
ATOM	733 CB LEU A 403	0.157 54.309 134.499 1.00 49.14	С

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		127/371	
ATOM	734 CG LEU A 403	-1.143 54.414 133.705 1.00 50.00	С
ATOM	735 CD1 LEU A 403		С
ATOM	736 CD2 LEU A 403	-1.218 55.729 132.979 1.00 50.69	С
ATOM	737 N PHE A 404	1.320 51.014 133.299 1.00 48.71	N
ATOM	738 CA PHE A 404		С
ATOM	739 C PHE A 404	1.035 51.013 130.872 1.00 49.94	C
ATOM	740 O PHE A 404	1.593 51.449 129.875 1.00 50.84	0
ATOM	741 CB PHE A 404	1.939 48.961 131.983 1.00 48.34	C
ATOM	742 CG PHE A 404		C
ATOM		2.917 48.338 134.176 1.00 49.16	C
ATOM	744 CD2 PHE A 404	4.381 48.409 132.309 1.00 48.46	C
ATOM	745 CE1 PHE A 404	3.989 47.974 134.994 1.00 48.97	C C
ATOM	746 CE2 PHE A 404 747 CZ PHE A 404	5.438 48.054 133.130 1.00 48.15 5.245 47.831 134.468 1.00 47.67	C
ATOM ATOM	747 CZ PHE A 404 748 N ALA A 405	-0.277 50.939 131.000 1.00 51.36	N
ATOM	748 N ALA A 403		C
ATOM	750 C ALA A 405	-2.365 52.175 130.749 1.00 54.33	c
ATOM	751 O ALA A 405	-2.547 52.092 131.967 1.00 56.08	ŏ
ATOM	752 CB ALA A 405	-1.856 50.215 129.350 1.00 53.05	C
ATOM	753 N PRO A 406	-3.219 52.850 129.995 1.00 54.64	N
ATOM	754 CA PRO A 406	-4.366 53.602 130.483 1.00 54.88	С
ATOM	755 C PRO A 406	-5.275 52.556 131.109 1.00 55.66	С
ATOM	756 O PRO A 406	-5.948 52.873 132.087 1.00 58.90	Ο
ATOM	757 CB PRO A 406	-5.037 54.376 129.367 1.00 53.81	С
ATOM	758 CG PRO A 406	-4.033 54.176 128.275 1.00 54.41	С
ATOM	759 CD PRO A 406	-3.182 52.956 128.551 1.00 54.81	С
ATOM	760 N ASN A 407	-5.250 51.347 130.590 1.00 54.42	N
ATOM	761 CA ASN A 407	-6.030 50.281 131.148 1.00 54.72	С
ATOM	762 C ASN A 407	-5.158 49.201 131.762 1.00 55.68	C
ATOM	763 O ASN A 407		0
ATOM		-6.924 49.703 130.059 1.00 55.56	C
ATOM		-6.093 48.843 129.120 1.00 55.68	C
	766 OD1 ASN A 407		O N
ATOM	767 ND2 ASN A 407 768 N LEU A 408	-3.970 49.522 132.274 1.00 55.43	N
ATOM ATOM	769 CA LEU A 408		C
ATOM	770 C LEU A 408	-2.441 49.270 134.032 1.00 54.84	c
ATOM	771 O LEU A 408	-1.520 49.964 133.660 1.00 54.42	ŏ
ATOM	772 CB LEU A 408	-2.282 47.623 132.172 1.00 55.04	C
ATOM	773 CG LEU A 408	-1.389 46.584 132.848 1.00 54.56	Č
ATOM	774 CD1 LEU A 408	-2.143 45.735 133.845 1.00 53.43	С
ATOM	775 CD2 LEU A 408	-0.746 45.703 131.772 1.00 54.04	С
ATOM	776 N LEUA 409	-2.920 49.190 135.268 1.00 55.99	N
ATOM	777 CA LEU A 409	-2.287 49.971 136.344 1.00 55.11	С
ATOM	778 C LEU A 409	-1.816 49.041 137.434 1.00 55.12	С

128/371 -2.616 48¹.795 138.321 1.00 57.05 0 **ATOM** 779 O LEU A 409 C -3.328 50.959 136.781 1.00 54.28 **ATOM** 780 CB LEU A 409 C 781 CG LEU A 409 -3.147 51.968 137.874 1.00 55.28 ATOM C -1.724 52.458 138.053 1.00 56.18 782 CD1 LEU A 409 ATOM 783 CD2 LEU A 409 -3.999 53.209 137.569 1.00 55.71 C **ATOM** N -0.608 48.499 137.370 1.00 55.36 **ATOM** 784 N LEU A 410 C 785 CA LEU A 410 -0.172 47.598 138.422 1.00 56.40 **ATOM** C 0.221 48.429 139.634 1.00 58.86 ATOM 786 C LEU A 410 0.460 49.643 139.561 1.00 59.46 0 787 O LEU A 410 ATOM C 788 CB LEU A 410 0.933 46.656 137.991 1.00 54.82 ATOM 789 CG LEU A 410 C 0.558 45.942 136.687 1.00 54.21 ATOM 790 CD1 LEU A 410 1.681 45.031 136.207 1.00 54.45 C **ATOM** C -0.733 45.192 136.922 1.00 53.26 791 CD2 LEU A 410 ATOM 792 N ASP A 411 0.223 47.704 140.730 1.00 60.91 N **ATOM** 0.543 48.300 142.026 1.00 64.05 C 793 CA ASP A 411 ATOM 1.813 47.646 142.525 1.00 63.96 C 794 C ASP A 411 ATOM 795 O ASP A 411 2.061 46.481 142.172 1.00 63.71 0 **ATOM** 796 CB ASP A 411 -0.721 48.022 142.835 1.00 68.11 C **ATOM** C 797 CG ASP A 411 -0.415 47.770 144.298 1.00 71.79 ATOM 798 OD1 ASP A 411 0.217 46.705 144.523 1.00 73.88 0 ATOM 799 OD2 ASP A 411 -0.793 48.646 145.116 1.00 73.30 0 **ATOM** 800 N ARG A 412 2.612 48.326 143.354 1.00 64.12 N ATOM 3.862 47.709 143.787 1.00 64.43 C 801 CA ARG A 412 ATOM C 802 C ARG A 412 3.761 46.216 144.061 1.00 65.36 ATOM 4.413 45.368 143.449 1.00 65.53 0 ATOM 803 O ARG A 412 4.473 48.394 144.996 1.00 63.99 C 804 CB ARG A 412 ATOM C ATOM 805 CG ARG A 412 5.476 47.466 145.681 1.00 64.51 6.364 48.216 146.642 1.00 65.90 C 806 CD ARG A 412 ATOM 7.612 47.514 146.947 1.00 66.08 807 NE ARG A 412 N ATOM 7.631 46.359 147.595 1.00 66.60 C 808 CZ ARG A 412 ATOM 809 NH1 ARG A 412 6.489 45.798 147.977 1.00 66.50 N ATOM N **ATOM** \$10 NH2 ARG A 412 8.794 45.782 147.852 1.00 67.25 2.936 45.816 145.001 1.00 66.84 N 811 N ASN A 413 ATOM 2.798 44.419 145.363 1.00 69.21 C 812 CA ASN A 413 ATOM 813 C ASN A 413 2.524 43.498 144.218 1.00 69.03 C ATOM 2.983 42,348 144,280 1.00 69.61 0 814 O ASN A 413 ATOM C 815 CB ASN A 413 1.703 44.331 146.438 1.00 73.12 ATOM \$16 CG ASN A 413 2.124 45.327 147.524 1.00 76.06 C ATOM 0 817 OD1 ASN A 413 3.078 44.994 148.239 1.00 77.88 ATOM 1.452 46.472 147.569 1.00 76.66 N 818 ND2 ASN A 413 ATOM N 819 N GLN A 414 1.883 43.910 143.128 1.00 68.31 ATOM 1.642 43.008 141.997 1.00 67.98 C ATOM 820 CA GLN A 414 C \$21 C GLN A 414 2.953 42.619 141.323 1.00 67.67 ATOM 3.059 41.664 140.555 1.00 67.18 0 S22 O GLN A 414 ATOM 0.647 43.591 141.021 1.00 68.30 C ATOM S23 CB GLN A 414

wo	98/56812	130/371	PCT/GB98/01708
ATOM	869 C MET A 421	10.198 43.267 140.603 1.00 60.86	С
ATOM		10.126 44.429 140.222 1.00 61.61	Ο
ATOM		9.053 41.763 139.110 1.00 63.01	С
ATOM		9.155 41.484 137.618 1.00 64.57	
ATOM		8.600 42.941 136.721 1.00 65.96	S
ATOM		6.843 42.583 136.658 1.00 65.26	С
ATOM		9.991 42.978 141.865 1.00 59.84	N
ATOM		9.671 43.990 142.842 1.00 59.34	С
ATOM	877 C VAL A 422	10.763 45.031 142.941 1.00 58.27	С
ATOM	878 O VAL A 422	10.400 46.177 143.150 1.00 58.27	0
		9.513 43.477 144.290 1.00 60.52	С
ATOM		8.283 44.098 144.911 1.00 59.97	С
ATOM		9.511 41.954 144.331 1.00 62.39	С
ATOM		12.014 44.624 142.845 1.00 57.88	N
ATOM		13.093 45.582 143.002 1.00 58.53	C
ATOM		13.054 46.565 141.842 1.00 56.03	С
ATOM		13.268 47.771 142.015 1.00 56.14	0
ATOM	886 CB GLU A 423	14.465 44.939 143.057 1.00 63.31	С
ATOM	887 CG GLU A 423	14.635 43.901 144.141 1.00 69.88	С
ATOM	888 CD GLU A 423	14.211 42.522 143.622 1.00 74.05	C
ATOM	889 OE1 GLU A 423	12.986 42.214 143.553 1.00 74.81	O
ATOM		15.172 41.762 143.287 1.00 76.76	Ο
ATOM		12.801 45.987 140.672 1.00 52.17	N
ATOM		12.714 46.851 139.483 1.00 49.13	C
ATOM		11.538 47.787 139.678 1.00 48.36	С
ATOM		11.673 49.013 139.527 1.00 48.89	0
ATOM		12.648 45.948 138.262 1.00 48.08	C
ATOM		13.983 45.195 138.186 1.00 47.42	C
ATOM	897 CG2 ILE A 424	12.405 46.751 137.013 1.00 48.16	C
ATOM		13.943 44.144 137.105 1.00 47.58	С
ATOM	899 N PHE A 425	10.384 47.274 140.097 1.00 46.94	N
ATOM	900 CA PHE A 425	9.231 48.116 140.345 1.00 47.55	C
ATOM			C
	902 O PHE A 425		0
	903 CB PHE A 425		C
	904 CG PHE A 425		C
	905 CD1 PHE A 425		C
ATOM			C
ATOM			C
ATOM		5.038 45.994 139.058 1.00 49.20	C C
ATOM		5.557 45.670 137.808 1.00 48.67	
ATOM		10.341 48.806 142.386 1.00 50.36	N C
	911 CA ASP A 426		C
	912 C ASP A 426		
ATOM	913 O ASP A 426	11.176 52.085 143.041 1.00 49.63	О

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ATOM	914 CB ASP A 426	11.406 48.954 144.534 1.00 53.65	С
ATOM	915 CG ASP A 426	10.316 48.430 145.473 1.00 56.55	C
ATOM	916 OD1 ASP A 426	9.170 48.940 145.384 1.00 57.43	Ō
ATOM	917 OD2 ASP A 426	10.590 47.529 146.301 1.00 58.16	Ö
ATOM	918 N MET A 427	12.575 50.575 142.083 1.00 49.66	N
ATOM	919 CA MET A 427	13.396 51.606 141.438 1.00 47.62	C
ATOM	920 C MET A 427	12.538 52.483 140.529 1.00 46.03	C
ATOM	921 O MET A 427	12.679 53.726 140.504 1.00 44.60	Ō
ATOM	922 CB MET A 427	14.476 50.885 140.655 1.00 48.02	C
ATOM	923 CG MET A 427	15.467 50.239 141.617 1.00 49.42	C
ATOM	924 SD MET A 427	16.870 49.639 140.649 1.00 51.75	S
ATOM	925 CE MET A 427	16.149 48.109 140.031 1.00 50.74	C
ATOM	926 N LEU A 428	11.627 51.786 139.817 1.00 43.62	N
ATOM	927 CA LEU A 428	10.719 52.557 138.954 1.00 43.05	С
ATOM	928 C LEU A 428	9.879 53.529 139.779 1.00 43.69	С
ATOM	929 O LEU A 428	9.804 54.738 139.487 1.00 43.73	Ο
ATOM	930 CB LEU A 428	9.884 51.598 138.134 1.00 41.42	С
ATOM	931 CG LEU A 428	10.630 50.884 137.008 1.00 39.99	С
ATOM	932 CD1 LEU A 428	9.754 49.788 136.444 1.00 39.57	С
ATOM	933 CD2 LEU A 428	11.004 51.865 135.920 1.00 40.09	С
ATOM	934 N LEU A 429	9.262 53.032 140.866 1.00 43.31	N
ATOM	935 CA LEU A 429	8.457 53.947 141.688 1.00 4 2 .48	С
ATOM	936 C LEU A 429	9.273 55.104 142.224 1.00 42.48	С
ATOM	937 O LEU A 429	8.897 56.281 142.110 1.00 42.82	Ο
ATOM	938 CB LEU A 429	7.725 53.158 142.761 1.00 41.76	С
ATOM	939 CG LEU A 429	6.674 52.197 142.202 1.00 41.28	C
ATOM	940 CD1 LEU A 429	6.320 51.130 143.211 1.00 42.51	C
ATOM	941 CD2 LEU A 429	5.404 52.920 141.801 1.00 41.15	С
ATOM	942 N ALA A 430	10.452 54.808 142.769 1.00 42.41	N
ATOM	943 CA ALA A 430	11.304 55.886 143.268 1.00 42.66	C
ATOM	944 C ALA A 430	11.554 56.960 142.217 1.00 43.57	C
ATOM	945 O ALA A 430	11.573 58.158 142.539 1.00 44.26	0
ATOM	946 CB ALA A 430	12.642 55.300 143.679 1.00 41.40	C
ATOM	947 N THR A 431	11.794 56.562 140.959 1.00 43.33	N
ATOM	948 CA THR A 431	12.075 57.589 139.956 1.00 44.07	C
ATOM	949 C THR A 431	10.814 58.382 139.711 1.00 45.04	C O
ATOM	950 O THR A 431	10.793 59.607 139.615 1.00 45.47 12.460 56.942 138.612 1.00 45.00	C
ATOM ATOM	951 CB THR A 431 952 OG1 THR A 431	13.421 55.921 138.929 1.00 46.49	O
ATOM	952 OG1 THR A 431 953 CG2 THR A 431	12.973 57.967 137.624 1.00 43.41	C
ATOM	954 N SER A 432	9.724 57.606 139.612 1.00 46.10	N
ATOM	955 CA SER A 432	8.414 58.218 139.367 1.00 47.08	C
ATOM		8.124 59.288 140.409 1.00 46.69	c
ATOM	957 O SER A 432	7.747 60.409 140.153 1.00 45.78	Õ
ATOM	958 CB SER A 432	7.350 57.120 139.344 1.00 47.86	C
7 F I O1VI	750 CD BERR 152	7,550 57,120 155,577 1.00 17,00	_

4.939 60.419 144.399 1.00 72.98

4.428 58.850 142.770 1.00 72.97

8.708 65.953 143.586 1.00 69.37

8.157 64.942 142.711 1.00 66.55

9.295 67.133 142.836 1.00 68.28

9.152 68.261 143.317 1.00 69.47

9.815 65.340 144.427 1.00 75.02

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997 NH1 ARG A 436

998 NH2 ARG A 436

999 N MET A 437

1000 CA MET A 437

1002 O MET A 437

ATOM 1001 C MET A 437

ATOM 1003 CB MET A 437

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ATOM	1049 CG GLU A 443	7.530 72.149 127.143 1.00 65.79	С
ATOM	1050 CD GLU A 443	6.392 71.931 128.137 1.00 68.13	С
		6.621 71.911 129.369 1.00 68.25	
ATOM	1052 OE2 GLU A 443	5.256 71.763 127.630 1.00 69.95	0
ATOM	1053 N GLU A 444	10.101 69.205 129.445 1.00 53.20	N
		11.331 68.677 130.012 1.00 51.24	
		11.397 67.171 129.727 1.00 50.05 12.444 66.683 129.258 1.00 50.87	
		11.372 68.890 131.514 1.00 50.94	
ATOM	1057 CB GLUA 444	11.572 08.890 131.314 1.00 30.94	C
ATOM	1059 CD GLU A 444	11.608 70.359 131.856 1.00 51.30 11.499 70.564 133.365 1.00 51.90	č
ATOM	1060 OE1 GLU A 444	10.606 69.965 134.020 1.00 51.11	Ö
		12.349 71.353 133.839 1.00 52.20	
ATOM	1062 N PHE A 445	10.282 66.481 129.989 1.00 46.38	N
ATOM	1063 CA PHE A 445	10.254 65.055 129.738 1.00 44.95	C
ATOM	1064 C PHE A 445	10.728 64.714 128.336 1.00 45.48	С
		11.613 63.901 128.118 1.00 47.22	
ATOM	1066 CB PHE A 445	8.844 64.523 129.927 1.00 43.54	С
ATOM	1067 CG PHE A 445	8.615 63.149 129.369 1.00 43.00 9.314 62.082 129.885 1.00 43.66	С
ATOM	1068 CD1 PHE A 445	9.314 62.082 129.885 1.00 43.66	C
ATOM	1069 CD2 PHE A 445	7.726 62.898 128.353 1.00 42.85	C
		9.132 60.799 129.421 1.00 44.24	
ATOM	10/1 CE2 PHE A 445	7.502 61.627 127.874 1.00 43.01	C
ATOM	1072 CZ FHE A 445	8.207 60.574 128.415 1.00 44.06 10.158 65.315 127.329 1.00 45.92	N
ATOM	1074 CA VALA 446	10.458 65.099 125.919 1.00 46.59	C
		11.915 65.347 125.625 1.00 48.14	
		12.579 64.661 124.811 1.00 49.23	
ATOM	1077 CB VAL A 446	9.400 65.935 125.178 1.00 46.86	С
ATOM	1078 CG1 VAL A 446	9.928 66.958 124.216 1.00 46.55 8.437 64.956 124.504 1.00 47.00	С
ATOM	1079 CG2 VAL A 446	8.437 64.956 124.504 1.00 47.00	
		12.545 66.323 126.279 1.00 48.23	N
	1081 CA CYS A 447	13.965 66.562 126.046 1.00 48.88	С
	1082 C CYS A 447	14.829 65.451 126.609 1.00 48.68	C
	1083 O CYS A 447 1084 CB CYS A 447	15.747 64.958 125.966 1.00 49.55	0
	1085 SG CYS A 447	14.346 67.868 126.761 1.00 50.37 13.962 69.266 125.693 1.00 54.72	C S
	1086 N LEU A 448	13.362 69.266 123.693 1.00 34.72	N N
	1087 CA LEU A 448	15.344 63.993 128.499 1.00 46.35	C
	1088 C LEU A 448	15.277 62.710 127.679 1.00 46.10	č
	1089 O LEU A 448	16.301 62.054 127.425 1.00 47.12	Ö
	1090 CB LEU A 448	14.819 63.712 129.882 1.00 47.13	C
ATOM	1091 CG LEU A 448	15.095 64.717 130.993 1.00 48.03	С
ATOM	1092 CD1 LEU A 448		С
ATOM	1093 CD2 LEU A 448	16.577 64.837 131.306 1.00 47.62	С

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ATOM	1130	CD1 LEU A 454	20.109 63.428 120.129 1.00 44.81	С
		CD2 LEU A 454	21.318 61.594 118.982 1.00 45.23	Ċ
		N ASN A 455	22.533 59.909 123.869 1.00 45.07	N
		CA ASN A 455	23.768 59.745 124.627 1.00 45.73	С
		C ASN A 455	24.057 58.330 125.013 1.00 48.44	С
ATOM	144	O ASN A 455	25.233 58.024 125.199 1.00 49.87	Ο
		CB ASN A 455	23.746 60.663 125.831 1.00 44.63	C
			24.714 60.421 126.940 1.00 45.06	C
			24.312 59.878 127.981 1.00 46.01	O N
		ND2 ASN A 455	25.991 60.781 126.797 1.00 45.17 23.085 57.454 125.143 1.00 51.91	N
		N SER A 456	23.403 56.111 125.615 1.00 51.70	C
		CA SER A 456 C SER A 456	24.368 55.318 124.791 1.00 57.99	c
		O SER A 456	25.335 54.734 125.316 1.00 60.18	Ö
			22.100 55.365 125.871 1.00 54.27	C
			21.657 55.684 127.170 1.00 53.76	Ο
		N GLY A 457	24.209 55.221 123.492 1.00 60.97	N
ATOM			25.128 54.406 122.689 1.00 63.92	С
ATOM		C GLY A 457	26.251 55.182 122.043 1.00 65.28	C
ATOM		O GLY A 457	26.903 54.604 121.187 1.00 64.24	0
ATOM		N VAL A 458	26.452 56.434 122.446 1.00 68.49	N
ATOM		CA VAL A 458	27.515 57.233 121.845 1.00 71.65	C
ATOM		C VAL A 458	28.920 56.730 122.068 1.00 75.14	C O
ATOM		O VAL A 458	29.697 56.796 121.100 1.00 75.96 27.347 58.721 122.178 1.00 70.32	C
		CB VAL A 458 CG1 VAL A 458	27.735 59.077 123.578 1.00 69.38	C
		CG2 VAL A 458	28.178 59.499 121.170 1.00 70.62	Č
		N TYR A 459	29.336 56.161 123.184 1.00 79.44	N
		CA TYR A 459	•	С
			30.891 54.266 122.826 1.00 86.75	С
ATOM	1169	O TYR A 459		Ο
ATOM	1170	CB TYR A 459	31.027 55.534 124.928 1.00 85.49	C
ATOM		CG TYR A 459	30.785 56.916 125.494 1.00 88.05	C
ATOM		CD1 TYR A 459	29.476 57.240 125.806 1.00 89.05	C
		CD2 TYR A 459	31.737 57.903 125.681 1.00 89.13	C C
		CE1 TYR A 459	29.259 58.504 126.266 1.00 90.57	C
		CE2 TYR A 459 CZ TYR A 459	31.444 59.165 126.177 1.00 90.01 30.152 59.486 126.502 1.00 91.08	c
		OH TYR A 459	29.680 60.685 127.003 1.00 92.07	Ö
		N THR A 460	30.044 53.813 121.918 1.00 89.04	N
		CA THR A 460	30.135 52.479 121.354 1.00 91.44	C
		C THR A 460	29.764 52.501 119.880 1.00 92.95	С
ATOM		O THR A 460	29.011 51.660 119.381 1.00 93.70	0
ATOM		2 CB THR A 460	29.206 51.507 122.105 1.00 91.84	С
ATOM	1183	OG1 THR A 460	28.435 52.146 123.118 1.00 92.33	0
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ATOM	1184	CG2 THR A 460	30.036 50.433 122.802 1.00 93.11	С
ATOM	1185	N PHE A 461	30.293 53.485 119.156 1.00 94.66	N
ATOM	1186	CA PHE A 461	29.937 53.571 117.743 1.00 95.99	С
ATOM	1187	C PHE A 461	30.457 52.502 116.795 1.00 97.27	С
ATOM	1188	O PHE A 461	29.707 52.075 115.884 1.00 97.97	Ο
ATOM	1189	CB PHE A 461	30.195 55.012 117.234 1.00 95.00	С
ATOM	1190	CG PHE A 461	28.849 55.690 117.222 1.00 93.86	С
ATOM	1191	CD1 PHE A 461	27.708 54.934 117.036 1.00 93.38	С
ATOM	1192	CD2 PHE A 461	28.725 57.045 117.407 1.00 94.19	С
ATOM	1193	CE1 PHE A 461	26.467 55.505 117.024 1.00 93.79	С
ATOM	1194	CE2 PHE A 461	27.478 57.635 117.393 1.00 94.10	С
ATOM	1195	CZ PHE A 461	26.349 56.866 117.199 1.00 94.05	С
ATOM	1196	N THR A 465	35.765 54.719 111.803 1.00128.15	N
ATOM	1197	CA THR A 465	36.448 55.536 112.810 1.00128.00	С
ATOM	1198	C THR A 465	36.314 57.024 112.518 1.00126.85	С
ATOM	1199	O THR A 465	35.594 57.732 113.235 1.00127.19	О
ATOM	1200	CB THR A 465	37.934 55.169 112.971 1.00128.63	С
ATOM	1201	OG1 THR A 465	38.671 56.294 113.484 1.00128.85	C
ATOM	1202	CG2 THR A 465	38.536 54.747 111.634 1.00128.96	C
ATOM	1203	N LEU A 466	36.948 57.527 111.457 1.00124.68	N
ATOM	1204	CA LEU A 466	36.834 58.946 111.109 1.00122.36	С
ATOM	.1205	C LEU A 466	35.380 59.372 110.897 1.00120.14	С
ATOM	1206	O LEU A 466	35.004 60.513 111.209 1.00120.35	О
ATOM	1207	CB LEU A 466	37.690 59.272 109.888 1.00122.63	С
ATOM	1211	N LYS A 467	34.533 58.469 110.392 1.00116.55	N
ATOM	1212	CA LYS A 467	33.110 58.730 110.232 1.00112.66	С
ATOM	1213	C LYS A 467	32.523 58.682 111.649 1.00108.51	С
		O LYS A 467		0
		CB LYS A 467		С
			31.105 58.236 108.677 1.00115.22	С
			30.310 57.054 108.135 1.00116.49	C
			30.421 56.878 106.630 1.00117.28	С
			29.774 55.614 106.152 1.00117.07	N
ATOM	1220	N SER A 468	33.064 57.846 112.522 1.00103.37	N
ATOM	1221	CA SER A 468	32.609 57.753 113.889 1.00 99.63	С
ATOM	1222	C SER A 468	32.923 59.038 114.652 1.00 96.39	C
ATOM	1223	O SER A 468	32.132 59.534 115.442 1.00 95.91	0
ATOM	1224	CB SER A 468	33.292 56.622 114.662 1.00100.41	C
ATOM	1225	OG SER A 468	32.848 55.358 114.205 1.00101.46	Ο
ATOM	1226	N LEU A 469	34.110 59.577 114.391 1.00 92.71	N
ATOM		CA LEU A 469	34.540 60.806 115.050 1.00 89.37	C
ATOM		C LEU A 469	33.583 61.906 114.627 1.00 86.96	C
ATOM	1229	O LEU A 469	33.213 62.769 115.417 1.00 86.78	0
ATOM		CB LEU A 469	36.009 61.096 114.755 1.00 89.59	С
ATOM	1234	N GLU A 470	33.150 61.868 113.379 1.00 84.76	N

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ATOM	1235 CA GLU A 470	32.201 62.860 112.869 1.00 83.39	С
ATOM	1236 C GLU A 470	30.812 62.559 113.408 1.00 79.41	С
ATOM	1237 O GLU A 470	30.032 63.445 113.738 1.00 78.64	Ο
ATOM	1238 CB GLU A 470	32.342 62.911 111.369 1.00 87.27	С
		31.065 62.883 110.562 1.00 92.97	С
		31.323 62.549 109.097 1.00 96.39	С
		32.446 62.061 108.788 1.00 98.06	0
	1242 OE2 GLU A 470		0
	1243 N GLU A 471		N
	1244 CA GLUA 471		C
	1245 C GLU A 471		C
		28.128 61.791 116.075 1.00 70.94 28.981 59.375 113.974 1.00 69.61	O C
ATOM	1247 CB GLUA 471	28.789 58.802 112.604 1.00 68.52	C
ATOM	1248 CO GLU A 471	27.388 58.530 112.148 1.00 68.47	C
		26.700 57.643 112.673 1.00 68.63	Ö
		26.838 59.174 111.232 1.00 68.52	Ö
	1252 N LYS A 472		N
	1253 CA LYS A 472	30.304 61.470 117.680 1.00 67.78	С
	1254 C LYS A 472	30.144 62.977 117.801 1.00 66.06	С
ATOM	1255 O LYS A 472	29.374 63.355 118.685 1.00 65.63	0
		31.582 61.016 118.375 1.00 69.03	С
ATOM	1257 CG LYS A 472	31.596 59.526 118.666 1.00 71.43	С
ATOM	1258 CD LYS A 472	32.719 59.148 119.613 1.00 74.06	C
		33.355 57.803 119.260 1.00 76.26	C
		32.614 56.637 119.848 1.00 77.74	N
	1261 N ASP A 473		N
	1262 CA ASP A 473	30.640 65.221 117.111 1.00 65.40 29.199 65.672 116.927 1.00 62.92	C C
ATOM	1203 C ASP A 473	28.600 66.391 117.720 1.00 63.45	0
ATOM		31.424 66.063 116.113 1.00 69.21	C
ATOM	1266 CG ASP A 473	32.907 65.839 116.318 1.00 73.72	Ċ
ATOM	1267 OD1 ASP A 473	33.269 65.168 117.325 1.00 76.19	0
	1268 OD2 ASP A 473	33.656 66.347 115.447 1.00 75.94	0
	1269 N HIS A 474	28.641 65.217 115.819 1.00 59.42	N
	1270 CA HIS A 474	27.262 65.532 115.494 1.00 55.77	C
ATOM	1271 C HIS A 474	26.393 65.294 116.722 1.00 54.86	С
	1272 O HIS A 474	25.647 66.153 117.187 1.00 53.76	О
	1273 CB HIS A 474	26.866 64.629 114.329 1.00 54.89	С
	1274 CG HIS A 474	25.458 65.016 113.979 1.00 55.54	C
	1275 ND1 HIS A 474	25.171 66.330 113.614 1.00 55.25	N
	1276 CD2 HIS A 474	24.313 64.286 113.980 1.00 55.43	C
ATOM	1277 CE1 HIS A 474	23.866 66.361 113.387 1.00 56.29	C
	1278 NE2 HIS A 474	23.320 65.149 113.598 1.00 55.98	N
ATUM	1279 N ILE A 475	26.480 64.088 117.288 1.00 54.45	N

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ATOM		23.049 71.538 123.043 1.00 52.02	С
		22.474 72.234 123.894 1.00 52.76	Ο
		25.530 71.463 122.818 1.00 52.27	
		26.854 70.920 123.300 1.00 53.57	
		26,911 70.289 124.371 1.00 54.43	0
		27.896 71.110 122.621 1.00 53.82	О
	1331 N LYS A 481		N
		21.331 72.106 121.440 1.00 54.53	
ATOM	1333 C LYS A 481	20.224 71.706 122.399 1.00 53.73	C
		19.568 72.572 122.972 1.00 54.44	0_
	1335 CB LYS A 481		C
		19.876 72.721 119.466 1.00 63.38	
	1337 CD LYS A 481		
		19.617 75.156 118.745 1.00 70.46	
		18.636 75.201 119.889 1.00 72.21	N
	1340 N ILE A 482		N
		18.973 69.958 123.549 1.00 50.20	С
		19.228 70.564 124.915 1.00 49.24	C
ATOM	1343 O ILE A 482	18.284 71.029 125.561 1.00 48.46	0
ATOM	1344 CB ILE A 482	18.795 68.444 123.582 1.00 49.95	С
ATOM	1345 CGITLE A 482	18.259 67.970 122.225 1.00 49.93	C
		17.788 67.989 124.619 1.00 49.78	C
		18.887 66.663 121.792 1.00 49.98	
	1348 N THR A 483		*
	1349 CA THR A 483	20.752 71.251 126.637 1.00 50.71 20.211 72.687 126.644 1.00 52.28	C C
	1350 C THR A 483 1351 O THR A 483	19.466 73.054 127.592 1.00 51.98	0
		22.260 71.245 126.953 1.00 49.92	C
		22.590 69.868 127.144 1.00 48.98	
	1354 CG2 THR A 483		
	1355 N ASP A 484	20.596 73.439 125.576 1.00 51.42	N
	1356 CA ASP A 484	20.142 74.829 125.467 1.00 50.56	Ċ
	1357 C ASP A 484	18.630 74.897 125.528 1.00 49.52	c
	1358 O ASP A 484	18.033 75.668 126.279 1.00 50.06	Ö
	1359 CB ASP A 484	20.661 75.526 124.233 1.00 51.89	C
	1360 CG ASP A 484	22.179 75.649 124.176 1.00 53.29	Ċ ·
	1361 OD1 ASP A 484	22.841 75.588 125.240 1.00 53.06	0
	1362 OD2 ASP A 484	22.706 75.807 123.039 1.00 53.68	Ō
	1363 N THR A 485	17.958 74.020 124.804 1.00 49.22	N
	1364 CA THR A 485	16.493 74.000 124.867 1.00 49.37	С
	1365 C THR A 485	16.010 73.836 126.288 1.00 50.25	С
	1366 O THR A 485	15.052 74.495 126.664 1.00 51.49	O
ATOM	1367 CB THR A 485	16.011 72.824 124.002 1.00 48.58	C
	1368 OG1 THR A 485	16.663 73.087 122.735 1.00 48.26	0
ATOM	1369 CG2 THR A 485	14.507 72.817 123.930 1.00 47.80	С

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ATOM	1370 N LEU A 486	16.646 72.984 127.084 1.00 51.08	N
ATOM	1371 CA LEU A 486	16,235 72.755 128.462 1.00 50.84	С
ATOM	1372 C LEU A 486	16.336 74.020 129.300 1.00 51.72	С
ATOM	1373 O LEU A 486	15.392 74.395 130.004 1.00 50.51	Ο
ATOM	1374 CB LEU A 486	17.083 71.660 129.124 1.00 48.86	С
ATOM	1375 CG LEU A 486	16.471 70.263 129.060 1.00 47.10	С
ATOM	1376 CD1 LEU A 486	17.415 69.268 129.691 1.00 45.88	С
ATOM	1377 CD2 LEU A 486	15.096 70.250 129.689 1.00 46.89	С
ATOM	1378 N ILE A 487	17.513 74.654 129.183 1.00 53.22	N
ATOM		17.705 75.893 129.962 1.00 55.44	С
	1380 C ILE A 487	16.687 76.950 129.526 1.00 57.52	C
	1381 O ILE A 487	16.035 77.649 130.299 1.00 57.79	0
ATOM		19.102 76.458 129.740 1.00 54.89	C
ATOM		20.160 75.546 130.329 1.00 55.18	C
		19.110 77.846 130.342 1.00 55.82	C
	1385 CD1 ILE A 487	20.418 75.650 131.804 1.00 54.44	C
	1386 N HIS A 488	16.531 77.063 128.204 1.00 59.32	N
ATOM	1387 CA HIS A 488	15.571 77.978 127.629 1.00 60.40	C C
ATOM	1388 C HIS A 488	14.232 77:757 128.321 1.00 59.31 13.649 78.686 128.844 1.00 60.16	0
ATOM	1389 O HIS A 488 1390 CB HIS A 488	15.408 77.680 126.142 1.00 63.58	C
	1391 CG HIS A 488	14.246 78.450 125.585 1.00 67.04	C
	1392 ND1 HIS A 488	14.282 79.820 125.450 1.00 68.39	N
		13.025 78.034 125.163 1.00 68.41	C
	1394 CE1 HIS A 488		č
ATOM		12.335 79.151 124.751 1.00 69.52	N
	1396 N LEU A 489	13.736 76.538 128.329 1.00 58.27	N
	1397 CA LEU A 489	12.481 76.237 128.963 1.00 58.66	С
ATOM	1398 C LEU A 489	12.402 76.732 130.400 1.00 59.58	С
ATOM	1399 O LEU A 489	11.403 77.276 130.854 1.00 59.17	Ο
ATOM	1400 CB LEU A 489	12.311 74.713 128.965 1.00 58.09	C
ATOM	1401 CG LEU A 489	11.844 74.125 127.647 1.00 58.45	C
ATOM	1402 CD1 LEU A 489	12.022 72.613 127.653 1.00 59.37	С
	1403 CD2 LEU A 489	10.381 74.471 127.412 1.00 59.03	С
	1404 N MET A 490	13.449 76.507 131.175 1.00 61.06	N
	1405 CA MET A 490	13.534 76.844 132.581 1.00 62.01	С
	1406 C MET A 490	13.545 78.337 132.851 1.00 62.91	C
	1407 O MET A 490	12.912 78.802 133.806 1.00 64.21	0
	1408 CB MET A 490	14.828 76.267 133.171 1.00 62.02	C
	1409 CG MET A 490	14.631 74.896 133.800 1.00 62.27	C
	1410 SD MET A 490	16.240 74.108 133.935 1.00 63.57	S C
	1411 CE MET A 490	15.813 72.389 133.645 1.00 63.55	
	1412 N ALA A 491	14.282 79.049 132.003 1.00 62.99	N
	1413 CA ALA A 491	14.346 80.503 132.143 1.00 63.54	C C
AIUM	1414 C ALA A 491	12.924 81.000 131.901 1.00 63.82	C

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ATOM	1415 () ALA A 491	12.370 81.706 132.732 1.00 63.44	0
ATOM		15.297 81.131 131.150 1.00 63.64	C
ATOM		12.293 80.539 130.827 1.00 64.75	N
	1418 CA LYS A 492	10.914 80.911 130.527 1.00 65.96	С
	1419 C LYS A 492	10.021 80.636 131.715 1.00 66.48	С
ATOM	1420 O LYS A 492	9.077 81.396 131.931 1.00 68.10	0
ATOM	1421 CB LYS A 492	10.378 80.274 129.245 1.00 66.21	С
ATOM	1426 N ALA A 493	10.251 79.654 132.568 1.00 67.14	N
ATOM	1427 CA ALA A 493	9.427 79.420 133.741 1.00 68.33	С
ATOM	1428 C ALA A 493	9.936 80.330 134.867 1.00 69.79	С
ATOM	1429 O ALA A 493	9.512 80.309 136.034 1.00 70.80	0
	1430 CB ALA A 493	9.451 77.976 134.198 1.00 68.17	С
	1431 N GLY A 494	10.904 81.171 134.533 1.00 70.02	N
	1432 CA GLY A 494	11.503 82.121 135.424 1.00 70.56	С
	1433 C GLY A 494	12.186 81.486 136.606 1.00 70.48	С
	1434 O GLY A 494	11.743 81.753 137.723 1.00 71.77	О
	1435 N LEU A 495	13.210 80.665 136.388 1.00 70.08	N
	1436 CA LEU A 495	13.898 80.138 137.574 1.00 69.07	С
	1437 C LEU A 495	15.184 80.965 137.611 1.00 69.25	C
	1438 O LEU A 495	15.641 81.270 136.500 1.00 69.64	0
	1439 CB LEU A 495	14.322 78.702 137.497 1.00 68.82	C
	1440 CG LEU A 495	13.325 77.646 137.061 1.00 68.59	C
	1441 CD1 LEU A 495	13.911 76.265 137.307 1.00 68.14	. C
	1442 CD2 LEU A 495	12.019 77.824 137.802 1.00 69.34	C
	1443 N THR A 496	15.704 81.275 138.775 1.00 69.48	N C
	1444 CA THR A 496 1445 C THR A 496	16.970 82.025 138.757 1.00 70.96 18.014 81.334 137.905 1.00 71.12	C
	1446 O THR A 496	17.950 80.134 137.620 1.00 72.23	0
	1447 CB THR A 496		C
		16.519 82.393 141.074 1.00 73.47	0
	1449 CG2 THR A 496	18.843 82.729 140.317 1.00 72.96	c
	1450 N LEU A 497	19.065 82.027 137.519 1.00 71.69	N
	1451 CA LEU A 497	20.155 81.450 136.753 1.00 72.39	C
	1452 C LEU A 497	20.770 80.305 137.571 1.00 72.97	Č
	1453 O LEU A 497	21.251 79.298 137.030 1.00 73.58	Ö
	1454 CB LEU A 497	21.204 82.515 136.508 1.00 73.26	С
ATOM	1455 CG LEU A 497	21.841 82,644 135,139 1.00 74.83	С
ATOM	1456 CD1 LEU A 497	23.368 82.634 135.296 1.00 74.97	С
ATOM	1457 CD2 LEU A 497	21.349 81.612 134.139 1.00 75.25	С
ATOM	1458 N GLN A 498	20.771 80.433 138.896 1.00 72.53	N
	1459 CA GLN A 498	21.320 79.378 139.727 1.00 72.61	С
ATOM	1460 C GLN A 498	20.306 78.254 139.801 1.00 71.51	С
ATOM	1461 O GLN A 498	20.710 77.090 139.784 1.00 72.93	Ο
ATOM	1462 CB GLN A 498	21.699 79.865 141.117 1.00 75.13	С
ATOM	1463 CG GLN A 498	21.645 78.783 142.173 1.00 78.79	C

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ATOM	1509 N ARG A 503	18.556 72.607 138.574 1.00 50.84	N
ATOM		17.570 71.742 137.948 1.00 49.11	С
ATOM	1511 C ARG A 503	18.224 70.926 136.833 1.00 48.91	С
ATOM	1512 O ARG A 503	18.000 69.712 136.750 1.00 51.21	0
ATOM	1513 CB ARG A 503	16.434 72.514 137.261 1.00 48.05	С
ATOM	1514 CG ARG A 503	15.201 71.634 137.089 1.00 46.69	С
ATOM	1515 CD ARG A 503	13.958 72.465 136.865 1.00 45.33	С
ATOM	1516 NE ARG A 503	12.869 71.641 136.368 1.00 46.09	N
ATOM	1517 CZ ARG A 503	11.992 70.959 137.112 1.00 46.32	С
ATOM	1518 NH1 ARG A 503	12.076 70.988 138.438 1.00 45.38	N
ATOM	1519 NH2 ARG A 503	11.022 70.243 136.533 1.00 45.97	N
ATOM	1520 N LEU A 504	19.020 71.592 136.000 1.00 46.31	N
ATOM	1521 CA LEU A 504	19.671 70.862 134.922 1.00 45.01	С
ATOM	1522 C LEU'A 504	20.351 69.636 135.509 1.00 45.72	С
ATOM	1523 O LEU A 504	20.031 68.494 135.196 1.00 46.55	O
ATOM	1524 CB LEU A 504	20.701 71.708 134.184 1.00 42.72	С
ATOM	1525 CG LEU A 504	21.245 71.069 132.910 1.00 41.21	С
	1526 CD1 LEU A 504	20.175 70.645 131.929 1.00 39.03	С
ATOM	1527 CD2 LEU A 504	22,269 72,018 132,296 1.00 41.69	С
	1528 N ALA A 505	21.284 69.921 136.418 1.00 46.05	N
		22.020 68.842 137.071 1.00 45.12	С
	1530 C ALA A 505	21.039 67.884 137.720 1.00 46.07	С
	1531 O ALA A 505	21.214 66.659 137.531 1.00 47.92	0
		23.023 69.450 138.011 1.00 43.45	С
		19.999 68.330 138.426 1.00 45.79	N
ATOM	1534 CA GLN A 506	19.110 67.322 139.006 1.00 47.26	С
ATOM	1535 C GLN A 506	18.472 66.448 137.940 1.00 47.55	С
	1536 O GLN A 506	18.349 65.234 138.187 1.00 48.38	0
		18.075 67.845 140.001 1.00 48.39	С
		18.389 69.172 140.639 0.50 50.04	С
		18.778 68.216 141.328 0.50 47.76	С
	1540 CD AGLN A 506	17.416 69.734 141.642 0.50 50.64	С
	1541 CD BGLN A 506	19.110 67.009 142.176 0.50 47.69	C
	1542 OE1AGLN A 506		0
	1543 OE1BGLN A 506		0
	1544 NE2AGLN A 506		N
	1545 NE2BGLN A 506	19.941 67.142 143.194 0.50 46.36	N
	1546 N LEU A 507	18.084 67.008 136.804 1.00 47.58	N
	1547 CA LEU A 507	17.459 66.207 135.760 1.00 47.73	C
	1548 C LEU A 507	18.407 65.182 135.162 1.00 47.79	C
	1549 O LEU A 507	18.096 63.974 135.131 1.00 49.51	Ō
	1550 CB LEU A 507	16.882 67.108 134.685 1.00 48.50	C
	1551 CG LEU A 507	15.653 67.920 135.116 1.00 48.92	Č
	1552 CD1 LEU A 507	15.253 68.828 133.952 1.00 50.13	C
	1553 CD2 LEU A 507	14.525 67.009 135.551 1.00 48.10	Ċ

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ΔΤΩΜ	1554	N LEU A 508	19.567 65.615 134.707 1.00 46.56	N
		CA LEU A 508	20.567 64.717 134.132 1.00 44.95	C
		C LEU A 508	21.067 63.710 135.148 1.00 44.15	С
		O LEU A 508	21.378 62.581 134.708 1.00 45.36	Ο
		CB LEU A 508	21.720 65.557 133.551 1.00 44.88	C
		CG LEU A 508	21.283 66.552 132.472 1.00 44.46	С
ATOM	1560	CD1 LEU A 508	22.431 67.354 131.935 1.00 44.78	С
		CD2 LEU A 508	20.679 65.822 131.280 1.00 46.15	C
		N LEU A 509	21.128 63.978 136.459 1.00 42.06	N
		CA LEU A 509	21.579 62.893 137.340 1.00 42.07	С
		C LEU A 509	20.557 61.753 137.417 1.00 42.29	C
		O LEU A 509	20.954 60.618 137.723 1.00 42.42	0
		CB LEU A 509	21.964 63.302 138.749 1.00 41.22	C C
ATOM	1567	CG LEU A 509	23.239 64.117 138.912 1.00 40.99	C
			23.332 64.611 140.339 1.00 40.83 24.439 63.279 138.525 1.00 39.70	C
		CD2 LEU A 509 N ILE A 510	19.275 61.989 137.116 1.00 42.24	N
			18.297 60.895 137.110 1.00 42.89	C
		C ILE A 510		c
		O ILE A 510		Ö
			16.841 61.359 137.037 1.00 42.87	C
ATOM	1575	CG1 ILE A 510	16.335 61.760 138.439 1.00 44.12	C
ATOM	1576	CG2 ILE A 510	15.874 60.297 136.573 1.00 42.19	С
		CD1 ILE A 510	15.616 63.111 138.389 1.00 45.79	C
		N LEUA511	19.196 60.421 134.908 1.00 40.88	N
			19.551 59.554 133.800 1.00 42.29	С
		C LEU A 511		С
		O LEUA511		0
ATOM	1582	CB LEU A 511	20.138 60.345 132.646 1.00 42.79	C
ATOM	1583	CG LEU A 511	19.232 61.427 132.042 1.00 42.59	С
ATOM	1584	CD1 LEU A 511	19.905 61.905 130.754 1.00 42.80	C
			17.832 60.894 131.792 1.00 41.41 21.353 58.661 135.190 1.00 42.45	N ·
		N SER A 512 CA SER A 512	22.199 57.597 135.692 1.00 42.43	C
		C SER A 512	21.372 56.441 136.243 1.00 41.74	c
ATOM	1589		21.593 55.272 135.918 1.00 41.94	Ö
		CB SER A 512	22.949 58.205 136.883 1.00 42.66	C
		OG SER A 512	24.235 57.651 136.722 1.00 46.60	Ö
ATOM		N HIS A 513	20,399 56,796 137.105 1.00 40.14	N
ATOM		CA HIS A 513	19.529 55.785 137.693 1.00 38.64	С
ATOM		C HIS A 513	18.762 55.039 136.606 1.00 39.44	С
	1595	O HIS A 513	18.646 53.790 136.644 1.00 39.11	0
		CB HIS A 513	18.604 56.417 138.732 1.00 37.52	С
ATOM		CG AHIS A 513	19.490 56.911 139.845 0.50 38.84	C
ATOM	1598	CG BHIS A 513	17.864 55.372 139.515 0.50 37.43	C

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		19.619 58.233 140.201 0.50 39.06	
ATOM	1600 ND1BHIS A 513	16.517 55.464 139.814 0.50 37.66	
ATOM	1601 CD2AHIS A 513	20.322 56.227 140.676 0.50 39.28	
		18.299 54.212 140.074 0.50 37.23	
	1603 CE1AHIS A 513		
ATOM	1604 CEIBHIS A 513	16.153 54.396 140.518 0.50 37.66	C
ATOM	1606 NE2RHIS A 513	20.919 57.143 141.514 0.50 38.49 17.217 53.622 140.689 0.50 37.60	N N
		8.281 55.782 135.589 1.00 38.07	N
		17.584 55.117 134.490 1.00 37.70	C
ATOM	1609 C ILE A 514 13	8.533 54.140 133.822 1.00 37.71	c
ATOM	1610 O ILE A 514 1	8.163 52.987 133.547 1.00 37.51	0
		16.950 56.154 133.575 1.00 38.13	С
		15.716 56.726 134.296 1.00 37.64	С
		16.570 55.603 132.205 1.00 38.53	
ATOM	1614 CD1 ILE A 514	15.430 58.128 133.808 1.00 37.44	С
		19.796 54.505 133.622 1.00 38.16	
		20.745 53.542 133.034 1.00 39.24 20.775 52.305 133.936 1.00 39.63	C C
		20.592 51.168 133.503 1.00 39.61	
		22.162 54.093 132.921 1.00 39.22	C
		23.163 53.364 132.063 1.00 40.21	Č
		22.636 53.155 130.689 1.00 44.06	С
		23.587 53.120 129.576 1.00 46.91	N
		24.178 54.247 129.165 1.00 48.77	
		23.949 55.429 129.752 1.00 49.82	
	1625 NH2 ARG A 515		N
		0.997 52.584 135.233 1.00 39.13	N
		21.081 51.538 136.221 1.00 38.90 9.936 50.555 136.121 1.00 39.18	C C
		0.140 49.355 135.970 1.00 37.84	0
		21.210 52.115 137.656 1.00 39.60	C
		21.440 50.946 138.595 1.00 39.71	C
ATOM	1632 ND1 HIS A 516	22.613 50.238 138.674 1.00 39.57	N
		20.608 50.321 139.453 1.00 39.43	С
		22.520 49.253 139.520 1.00 38.56	С
		21.300 49.283 140.017 1.00 38.92	N
		18.707 51.044 136.207 1.00 41.07	N
		17.480 50.261 136.129 1.00 41.63	C
		17.341 49.430 134.871 1.00 41.41 16.945 48.280 134.891 1.00 40.72	C 0
		16.298 51.237 136.037 1.00 42.72	C
		15.515 51.311 137.335 1.00 44.29	Č
	1642 SD MET A 517	14.274 52.640 137.213 1.00 45.43	S
ATOM	1643 CE MET A 517	15.401 54.009 137.346 1.00 47.82	С

		(4+1)3+1	
ATOM	1644 N SER A 518	17.681 50.082 133.758 1.00 42.10	N
ATOM	1645 CA SER A 518	17.638 49.441 132.446 1.00 42.47	С
	1646 C SER A 518	18.569 48.244 132.411 1.00 42.00	С
ATOM	1647 O SER A 518	18.200 47.199 131.873 1.00 42.03	0
ATOM	1648 CB SER A 518	18.007 50.484 131.407 1.00 43.32	С
ATOM	1649 OG SER A 518	18.544 49.964 130.228 1.00 45.64	0
ATOM	1650 N ASN A 519	19.748 48.392 132.990 1.00 42.37	N
ATOM	1651 CA ASN A 519	20.713 47.295 133.030 1.00 44.29	С
ATOM	1652 C ASN A 519	20.084 46.169 133.831 1.00 44.94	С
ATOM	1653 O ASN A 519	20.079 45.036 133.362 1.00 46.19	0
ATOM	1654 CB ASN A 519		С
	1655 CG ASN A 519	22.911 48.548 132.631 1.00 49.35	C
	1656 OD1 ASN A 519	22.901 48.175 131.438 1.00 51.40	Ο
	1657 ND2 ASN A 519	23.625 49.607 133.033 1.00 48.18	N
ATOM	1658 N LYS A 520	19.498 46.414 134.995 1.00 44.94	N
ATOM	1659 CA LYS A 520	18.871 45.362 135.763 1.00 45.92	С
ATOM	1660 C LYS A 520	17.671 44.792 135.027 1.00 46.12	С
ATOM	1661 O LYS A 520	17.453 43.581 135.088 1.00 46.63	Ο
ATOM	1662 CB LYS A 520	18.367 45.898 137.088 1.00 48.44	С
ATOM	1663 CG LYS A 520	19.437 46.800 137.700 1.00 50.91	С
ATOM	1664 CD LYS A 520	20.181 45.926 138.689 1.00 53.34	С
ATOM	1665 CE LYS A 520	21.647 45.782 138.339 1.00 55.85	С
ATOM	1666 NZ LYS A 520	22.201 44.573 139.041 1.00 58.02	N
ATOM	1667 N GLY A 521	16.918 45.665 134.365 1.00 45.54	N
ATOM	1668 CA GLY A 521	15.807 45.181 133.568 1.00 45.58	С
ATOM	1669 C GLY A 521	16.270 44.202 132.482 1.00 45.78	С
ATOM	1670 O GLY A 521	15.561 43.182 132.432 1.00 45.24	Ο
ATOM	1671 N MET A 522	17.328 44.439 131.676 1.00 45.68	N
ATOM	1672 CA MET A 522	17.660 43.456 130.663 1.00 46.96	С
ATOM	1673 C MET A 522	18.061 42.141 131.346 1.00 48.31	С
ATOM	1674 O MET A 522	17.612 41.095 130.901 1.00 48.01	О
ATOM	1675 CB MET A 522		С
ATOM	1676 CG MET A 522	19.335 44.821 129.041 1.00 47.52	C
ATOM	1677 SD MET A 522	18.355 45.460 127.700 1.00 48.79	S
ATOM	1678 CE MET A 522	17.616 43.967 127.040 1.00 46.55	С
ATOM	1679 N GLU A 523	18.909 42.283 132.369 1.00 49.71	N
ATOM	1680 CA GLU A 523	19.336 41.083 133.075 1.00 51.07	С
ATOM	1681 C GLU A 523	18.137 40.248 133.475 1.00 48.53	C
ATOM	1682 O GLU A 523	18.134 39.039 133.310 1.00 48.65	0
ATOM	1683 CB GLU A 523	20.203 41.486 134.239 1.00 57.61	C
ATOM	1684 CG GLU A 523	21.688 41.593 133.956 1.00 64.95	C
ATOM	1685 CD GLU A 523	22.270 40.403 133.199 1.00 69.95	C
ATOM	1686 OE1 GLU A 523	21.645 39.297 133.221 1.00 72.64	0
ATOM	1687 OE2 GLU A 523	23.373 40.581 132.589 1.00 72.19	. 0
ATOM	1688 N HIS A 524	17.075 40.836 133.978 1.00 46.39	N

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ATOM	1689 CA HIS A 524	15.865 40.144 134.344 1.00 45.35	С
ATOM	1690 C HIS A 524	15.097 39.606 133.156 1.00 45.66	С
ATOM	1691 O HIS A 524	14.678 38.453 133.149 1.00 45.67	0
ATOM	1692 CB HIS A 524	14.953 41.109 135.115 1.00 43.98	С
ATOM	1693 CG HIS A 524	13.627 40.538 135.470 1.00 43.57	С
ATOM	1694 ND1 HIS A 524	12.542 40.552 134.611 1.00 44.22	N
ATOM	1695 CD2 HIS A 524	13.185 39.925 136.580 1.00 43.73	С
ATOM	1696 CE1 HIS A 524	11.505 39.982 135.189 1.00 44.25	С
ATOM	1697 NE2 HIS A 524	11.855 39.579 136.402 1.00 43.68	N
ATOM	1698 N LEU A 525	14.873 40.389 132.110 1.00 47.35	N
ATOM	1699 CA LEU A 525	14.074 39.974 130.954 1.00 49.08	С
ATOM	1700 C LEU A 525	14.721 38.741 130.341 1.00 51.79	С
ATOM	1701 O LEUA 525	14.098 37.840 129.819 1.00 51.57	Ο
ATOM	1702 CB LEU A 525	13.912 41.078 129.907 1.00 47.41	С
ATOM	1703 CG LEU A 525	13.259 40.641 128.599 1.00 46.29	С
ATOM	1704 CD1 LEU A 525	11.822 40.216 128.816 1.00 45.85	С
ATOM	1705 CD2 LEU A 525	13.321 41.793 127.618 1.00 45.98	С
ATOM	1706 N TYR A 526	16.043 38.747 130.444 1.00 55.42	N
ATOM	1707 CA TYR A 526	16.912 37.700 129.978 1.00 58.28	С
ATOM	1708 C TYR A 526	16.695 36.442 130.791 1.00 58.73	С
ATOM	1709 O TYR A 526	16.532 35.382 130.189 1.00 59.67	Ο
ATOM	1710 CB TYR A 526	18.351 38.203 130.088 1.00 60.44	С
ATOM	1711 CG TYR A 526	19.231 37.154 129.479 1.00 63.65	С
ATOM	1712 CD1 TYR A 526	19.396 37.063 128.120 1.00 66.19	С
ATOM	1713 CD2 TYR A 526	19.864 36.252 130.293 1.00 66.21	С
ATOM	1714 CE1 TYR A 526		С
	1715 CE2 TYR A 526		С
	1716 CZ TYR A 526		С
ATOM		21.647 34.235 127.874 1.00 74.44	О
ATOM		16.663 36.506 132.116 1.00 59.86	N
ATOM		16.424 35.244 132.848 1.00 61.25	С
ATOM	1720 C SER A 527		C
		14.818 33.689 132.186 1.00 62.52	0
ATOM	1722 CB SER A 527	16.686 35.314 134.336 1.00 61.10	C
	1723 OG SER A 527	16.238 36.600 134.712 1.00 61.91	0
	1724 N MET A 528	14.008 35.720 132.619 1.00 62.93	N
	1725 CA MET A 528	12.643 35.385 132.249 1.00 63.77	C
	1726 C MET A 528	12.615 34.640 130.920 1.00 64.50	C
	1727 O MET A 528	11.878 33.669 130.756 1.00 63.77	0
ATOM	1728 CB MET A 528	11.800 36.650 132.126 1.00 64.26	C
ATOM	1729 CG MET A 528	11.182 37.186 133.395 1.00 64.61	C
	1730 SD MET A 528	10.838 35.959 134.659 1.00 65.93	S
	1731 CE MET A 528	12.311 36.036 135.659 1.00 64.66	C
	1732 N LYS A 529	13.400 35.038 129.935 1.00 66.98	N
ATOM	1733 CA LYS A 529	13.464 34.355 128.651 1.00 70.45	С

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ATOM	1734 C LYS A 529	14.098 32.973 128.783 1.00 72.45	С
ATOM		13.658 32.014 128.150 1.00 72.88	Ο
	1736 CB LYS A 529	14,256 35,190 127,655 1,00 71,06	С
		15.273 34.456 126.823 1.00 73.17	С
ATOM		15.124 34.855 125.362 1.00 76.29	С
ATOM	1739 CE LYS A 529		C
ATOM		17.601 34.302 125.151 1.00 80.14	N
ATOM		15.153 32.854 129.573 1.00 75.18	N
ATOM	1742 CA CYS A 530	15.829 31.576 129.772 1.00 78.32	C
ATOM	1743 C CYS A 530	14.945 30.584 130.490 1.00 80.30	c
ATOM			Ö
	1745 CB CYS A 530		Č
	1746 SG ACYS A 530	18.275 32.752 129.297 0.50 79.21	S
ATOM		17.568 30.622 131.680 0.50 81.24	S
ATOM		14.102 31.009 131.421 1.00 82.32	N
		13.144 30.200 132.155 1.00 83.76	C
	1750 C LYS A 531	11.970 29.841 131.246 1.00 85.00	c
	1751 O LYS A 531		ŏ
		12.572 30.964 133.355 1.00 83.88	C
ATOM		13.345 30.854 134.647 1.00 84.87	C
		14.805 31.287 134.574 1.00 85.69	C
ATOM		11.943 30.327 130.025 1.00 86.68	N
ATOM	1758 CA ASN A 532	10.897 30.076 129.057 1.00 88.62	C
		9.561 30.539 129.591 1.00 87.46	c
	1759 C ASN A 532 1760 O ASN A 532	8.631 29.761 129.724 1.00 88.90	o
ATOM		10.865 28.584 128.719 1.00 91.95	C
ATOM		12.111 28.192 127.933 1.00 95.44	C
	1762 CG ASN A 532	12.541 28.192 127.933 1.00 93.44	0
	1763 OD1 ASN A 532	12.541 28.919 127.018 1.00 97.13	N
	1764 ND2 ASN A 532	9.437 31.803 129.937 1.00 85.64	N
	1765 N VAL A 533		C
	1766 CA VAL A 533	7.754 33.510 129.545 1.00 83.66	c
ATOM		6.622 33.965 129.431 1.00 84.28	0
	1768 O VAL A 533	8.579 33.025 131.836 1.00 83.74	Č
	1769 CB VAL A 533		C
	1770 CG1 VAL A 533	7.314 33.478 132.539 1.00 84.23	C
	1771 CG2 VAL A 533	9.365 32.100 132.744 1.00 83.35	N
	1772 N VAL A 534	8.709 34.036 128.803 1.00 82.83	C
	1773 CA VAL A 534	8.538 35.100 127.846 1.00 82.58	C
	1774 C VAL A 534	8.243 34.525 126.465 1.00 82.12	
	1775 O VAL A 534	8.956 33.657 125.956 1.00 81.14	O C
	1776 CB VAL A 534	9.852 35.922 127.723 1.00 83.39	
	1777 CG1 VAL A 534	9.874 36.971 126.614 1.00 83.09	C C
	1778 CG2 VAL A 534	10.138 36.622 129.047 1.00 84.00	_
	1779 N PRO A 535	7.211 35.078 125.856 1.00 81.83	N
AIOM	1780 CA PRO A 535	6.814 34.762 124.508 1.00 82.27	С

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ATOM	1781 C PRO A 535	7.903 35.219 123.523 1.00 83.08	С
		8.852 35.993 123.727 1.00 81.80	0
ATOM	1783 CB PRO A 535	5.489 35.480 124.209 1.00 81.89	С
ATOM	1784 CG PRO A 535	5.161 36.150 125.500 1.00 81.49	С
ATOM	1785 CD PRO A 535	5.161 36.150 125.500 1.00 81.49 6.365 36.127 126.413 1.00 81.75	С
ATOM	1786 N LEU A 536	7.710 34.667 122.314 1.00 84.28	N
ATOM	1787 CA LEU A 536	8.585 34.888 121.181 1.00 84.76	С
ATOM	1788 C LEU A 536	8.321 36.144 120.362 1.00 83.94	С
ATOM	1789 O LEU A 536	8.224 36.055 119.125 1.00 84.95 8.213 37.297 121.028 1.00 81.31	O
			N
		7.998 38.516 120.254 1.00 78.44	C
ATOM	1796 C TYR A 537	9.356 38.798 119.616 1.00 76.32	С
ATOM	1797 O TYR A 537	10.358 38.868 120.302 1.00 74.82	0
ATOM	1798 CB TYR A 537	7.515 39.639 121.120 1.00 79.11 6.202 39.346 121.803 1.00 79.98	C
ATOM	1799 CG TYR A 537	6.202 39.346 121.803 1.00 79.98	C
ATOM	1800 CD1 TYR A 537	5.051 39.111 121.078 1.00 80.95	C
ATOM	1801 CD2 TYR A 537	6.097 39.316 123.180 1.00 80.52	C
ATOM	1802 CEI TYR A 537	3.834 38.849 121.682 1.00 81.26	С
ATOM	1803 CE2 TYR A 537	4.888 39.059 123.788 1.00 80.94 3.759 38.826 123.052 1.00 81.36	С
ATOM	1804 CZ TYR A 537	3.759 38.826 123.052 1.00 81.36	С
		2.544 38.569 123.656 1.00 81.97	0
		9.336 38.912 118.299 1.00 74.66	N C
		10.514 39.140 117.499 1.00 71.95 11.270 40.430 117.671 1.00 66.96	c
ATOM	1000 C ASP A 330	12.485 40.348 117.818 1.00 66.05	0
ATOM	1810 CR ASP A 538	10.065 39.019 116.029 1.00 77.04	C
		10.164 37.552 115.613 1.00 81.25	Č
		11.125 36.875 116.066 1.00 83.37	
		9.308 37.060 114.837 1.00 83.49	
ATOM	1814 N LEUA 539	10.635 41.587 117.635 1.00 61.63	N
		11.356 42.857 117.766 1.00 56.44	С
	1816 C LEU A 539	11.971 42.988 119.139 1.00 56.25	С
ATOM	1817 O LEUA 539	13.082 43.499 119.280 1.00 56.68	0
ATOM	1818 CB LEU A 539	10.416 44.005 117.465 1.00 54.10	С
ATOM	1819 CG LEU A 539	10.884 45.430 117.325 1.00 51.84	С
ATOM	1820 CD1 LEU A 539	12.181 45.567 116.558 1.00 52.42	С
	1821 CD2 LEU A 539	9.833 46.284 116.643 1.00 50.66	С
	1822 N LEUA 540	11.279 42.532 120.186 1.00 55.25	N
	1823 CA LEU A 540	11.747 42.556 121.561 1.00 52.61	С
	1824 C LEU A 540	12.920 41.597 121.684 1.00 52.69	C
	1825 O LEU A 540	13.927 41.999 122.263 1.00 53.12	0
ATOM	1826 CB LEU A 540	10.646 42.178 122.551 1.00 51.55	C
ATOM	1827 CG LEU A 540	10.979 42.209 124.044 1.00 50.31	С
ATOM		10.994 43.630 124.578 1.00 49.58	C
ATOM	1829 CD2 LEU A 540	10.015 41.374 124.860 1.00 49.08	С

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АТОМ	1920 C SER B 305	27.429 71.556 157.295 1.00 88.55	С
ATOM		27.225 72.515 156.538 1.00 88.16	Ō
		25.569 69.949 156.772 1.00 88.41	C
ATOM	1923 OG SER B 305	26.477 69.152 156.035 1.00 87.79	
	1924 N LEUB 306		N
	1925 CA LEU B 306	29.821 71.887 157.029 1.00 87.60	С
	1926 C LEUB 306		С
	1927 O LEUB 306		0
ATOM	1928 CB LEU B 306	31.152 71.166 157.258 1.00 88.10	С
	1932 N ALA B 307		N
		28.954 70.789 153.506 1.00 83.05	С
	1934 C ALA B 307		С
ATOM	1935 O ALA B 307	28.688 72.783 152.238 1.00 82.40	0
ATOM	1936 CB ALA B 307	28.050 69.587 153.251 1.00 83.80	С
ATOM	1937 N LEUB 308	27.028 72.255 153.665 1.00 81.16	N
	1938 CA LEUB 308	26.224 73.402 153.311 1.00 81.25	С
	1939 C LEUB 308		С
	1940 O LEUB 308		0
		24.833 73.206 153.918 1.00 80.91	С
		24.119 71.927 153.501 1.00 81.19	C
		22.625 72.029 153.804 1.00 82.22	C
		24.303 71.612 152.027 1.00 81.42	C
	1945 N SER B 309		N
	*	28.504 76.235 154.570 1.00 80.23	C
	1947 C SER B 309	29.757 76.570 153.798 1.00 78.85	C
ATOM	1948 O SER B 309	30.061 77.749 153.621 1.00 80.10	O C
ATOM		28.945 76.199 156.048 1.00 81.60	
		27.839 75.621 156.755 1.00 84.43 30.509 75.562 153.373 1.00 76.88	N
ATOM	1951 N LEUB 310	31.727 75.890 152.636 1.00 74.77	C
	1953 C LEUB 310		c
ATOM	1954 O LEUB 310	30.248 76.603 150.819 1.00 73.10	Ö
ATOM	1955 CB LEU B 310	32.577 74.676 152.338 1.00 74.13	Č .
ATOM	1956 CG LEU B 310	32.501 73.548 153.358 1.00 73.86	Č
ATOM	1957 CD1 LEU B 310	31.862 72.354 152.682 1.00 73.73	C
ATOM	1958 CD2 LEU B 310	33.893 73.207 153.878 1.00 74.39	C
ATOM	1959 N THR B 311	32.356 77.379 150.891 1.00 72.63	N
ATOM	1960 CA THR B 311	32.217 78.181 149.680 1.00 71.48	C
	1961 C THR B 311	32.717 77.311 148.556 1.00 70.23	С
	1962 O THR B 311	33.526 76.425 148.873 1.00 69.71	0
	1963 CB THR B 311	33.046 79.459 149.869 1.00 72.04	С
ATOM	1964 OG1 THR B 311	34.432 79.184 150.007 1.00 71.51	О
ATOM	1965 CG2 THR B 311	32.624 80.144 151.172 1.00 72.51	С
ATOM	1966 N ALA B 312	32.343 77.539 147.311 1.00 69.55	N
ATOM	1967 CA ALA B 312	32.847 76.686 146.239 1.00 69.89	C

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ATOM		34.355 76.490 146.399 1.00 70.66	С
ATOM		34.812 75.352 146.204 1.00 71.02	0
		32.533 77.194 144.852 1.00 69.74	C
	1971 N ASP B 313	35.109 77.532 146.738 1.00 71.01	N
	1972 CA ASP B 313	36.532 77.350 146.907 1.00 72.28	C
	1973 C ASP B 313	36.896 76.400 148.016 1.00 71.15	C O
	1974 O ASP B 313	37.776 75.572 147.780 1.00 70.97 37.207 78.709 147.104 1.00 76.97	C
ATOM	1975 CD ASP B 313	37.316 79.339 145.715 1.00 81.71	C
		37.885 78.667 144.807 1.00 83.39	Ö
		36,821 80.490 145.531 1.00 84.01	Ŏ
	1979 N GLNB 314	36.282 76.463 149.186 1.00 70.43	N
		36.617 75.551 150.272 1.00 70.03	C
	1981 C GLN B 314	36.258 74.111 149.897 1.00 68.40	С
		37.035 73.183 150.134 1.00 68.40	0
ATOM	1983 CB GLN B 314	35.863 75.933 151.539 1.00 72.10	С
		35.710 77.430 151.674 1.00 74.15	С
		35.109 77.833 153.005 1.00 75.96	С
		33.942 78.211 153.112 1.00 77.07	0
		35.968 77.728 154.015 1.00 76.35	N
	1988 N MET B 315	35.068 73.967 149.304 1.00 65.55	N
		34.585 72.674 148.838 1.00 62.07	
	1990 C MET B 315	35.664 72.028 147.976 1.00 60.02	С
	1991 O MET B 315 1992 CB MET B 315	36.124 70.920 148.247 1.00 58.85 33.289 72.894 148.070 1.00 61.80	O C
	1992 CB MET B 315	32.588 71.654 147.554 1.00 62.43	C
	1994 SD MET B 315		S
		32.375 69.332 148.932 1.00 62.81	
		36.101 72.735 146.936 1.00 58.75	N
		37.113 72.194 146.044 1.00 59.58	C
		38.356 71.690 146.767 1.00 60.61	С
ATOM	1999 O VAL B 316	38.881 70.619 146.456 1.00 61.28	0
ATOM	2000 CB VAL B 316	37.610 73.173 144.958 1.00 59.08	С
		38.727 72.541 144.132 1.00 58.28	С
		36.478 73.560 144.022 1.00 59.27	С
	2003 N SER B 317	38.877 72.498 147.672 1.00 61.25	N
	2004 CA SER B 317	40.097 72.148 148.395 1.00 61.71	C
	2005 C SER B 317	39.843 70.994 149.344 1.00 60.20	C
	2006 O SER B 317	40.676 70.092 149.474 1.00 60.58	0
	2007 CB SER B 317	40.539 73.355 149.236 1.00 64.18	C O
	2008 OG SER B 317 2009 N ALA B 318	39.510 74.345 149.098 1.00 67.30 38.668 71.040 149.975 1.00 57.91	N
	2010 CA ALA B 318	38.335 69.952 150.891 1.00 56.48	C
		38.428 68.646 150.098 1.00 55.76	c
	2012 O ALAB 318	38.992 67.662 150.580 1.00 55.85	Ö
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	2013 CB ALA B 318	36.946 70.127 151.461 1.00 56.32	С
	2014 N LEUB 319		N
		37.824 67.501 148.044 1.00 53.50	С
	2016 C LEUB 319	39.205 67.171 147.565 1.00 54.80	С
	2017 O LEUB 319		О
	2018 CB LEU B 319	36.878 67.720 146.888 1.00 51.65	С
		35,392 67,769 147,282 1.00 51.14	C
		34.606 68.162 146.040 1.00 50.92	C
	2021 CD2 LEU B 319	34.931 66.463 147.916 1.00 49.29	С
	2022 N LEUB 320	39.921 68.193 147.116 1.00 57.27	N
		41.298 68.008 146.647 1.00 58.44	С
	2024 C LEUB 320	42.131 67.387 147.747 1.00 60.71	С
	2025 O LEUB 320		О
		41.847 69.356 146.194 1.00 57.26	C
		41.571 69.548 144.707 1.00 57.56	С
		42.037 70.904 144.200 1.00 58.40	С
	•	42.260 68.415 143.954 1.00 57.16	С
	2030 N ASP B 321	41.848 67.748 148.988 1.00 63.60	N
		42.558 67.207 150.114 1.00 67.77	С
	2032 C ASP B 321	42.264 65.767 150.479 1.00 66.98	С
	2033 O ASP B 321	43.153 65.028 150.905 1.00 68.46	0
		42.159 68.035 151.346 1.00 73.48	C
		43.357 68.907 151.702 1.00 78.86	C
		44.358 68.838 150.933 1.00 80.91	0
	2037 OD2 ASP B 321	43.234 69.622 152.738 1.00 81.75	0
	2038 N ALA B 322	41.013 65.337 150.345 1.00 64.01	N
	2039 CA ALA B 322	40.651 63.979 150.713 1.00 60.43	С
	2040 C ALA B 322	41.260 62.949 149.783 1.00 59.13	C
	2041 O ALA B 322		0
		39.130 63.958 150.695 1.00 59.91	C
	2043 N GLUB 323		N
	2044 CA GLU B 323	42.265 62.393 147.650 1.00 56.07	С
ATOM		43.165 61.402 148.323 1.00 55.73	C
	2046 O GLUB 323	43.982 61.745 149.167 1.00 58.17	0
	2047 CB GLUB 323	42.959 63.161 146.539 1.00 56.37	C
ATOM		41.903 63.704 145.555 1.00 57.34	C
ATOM		41.427 62.553 144.690 1.00 58.29	C
ATOM		42.238 61.857 144.034 1.00 59.37	0
	2051 OE2 GLU B 323	40.222 62.286 144.663 1.00 58.17	0
	2052 N PRO B 324	43.009 60.136 148.013 1.00 55.05	N
	2053 CA PRO B 324	43.797 59.044 148.563 1.00 54.36	C
	2054 C PRO B 324	45.142 58.976 147.861 1.00 55.37	С
ATOM		45.401 59.613 146.835 1.00 56.48	0
	2056 CB PRO B 324	43.006 57.765 148.252 1.00 53.47	C
ATOM	2057 CG PRO B 324	42.269 58.183 147.016 1.00 53.95	С

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ATOM	2058 CD PRO B 324	42.056 59.670 146.998 1.00 54.63	С
ATOM	2059 N PRO B 325	46.032 58.173 148.383 1.00 55.73	N
ATOM	2060 CA PRO B 325	47.354 57.952 147.848 1.00 56.79 47.235 57.105 146.593 1.00 58.51	C
ATOM	2061 C PRO B 325	47.235 57.105 146.593 1.00 58.51	С
ATOM	2062 O PROB 325	46.186 56.455 146.548 1.00 59.42	0
		48.084 57.111 148.908 1.00 56.61	C
		46.945 56.405 149.583 1.00 56.03	С
		45.784 57.370 149.587 1.00 56.49	С
		48.185 57.070 145.677 1.00 59.89	N
		48.081 56.220 144.497 1.00 61.78	C
		48.771 54.904 144.848 1.00 60.68 49.919 55.033 145.279 1.00 62.66	
ATOM	2009 O ILEB 320	49.919 33.033 143.279 1.00 62.66	O C
ATOM	2070 CB ILEB 320	48.774 56.685 143.208 1.00 65.00 50.257 57.062 143.384 1.00 68.09	C
ATOM	2072 CG2 ILE B 326	48.016 57.832 142.521 1.00 64.84	
ATOM	2073 CD1 ILE B 326	50.668 57.986 144.527 1.00 69.81	č
	2074 N LEUB 327		N
		48.909 52.546 145.122 1.00 58.44	
		49.829 52.088 144.008 1.00 58.98	C
ATOM	2077 O LEUB 327	49.826 52.665 142.938 1.00 59.09	0
ATOM	2078 CB LEU B 327	47.876 51.501 145.502 1.00 57.19	С
ATOM	2079 CG LEUB 327	46.808 51.909 146.493 1.00 56.05	С
ATOM	2080 CD1 LEU B 327	46.233 50.637 147.122 1.00 55.97 47.321 52.844 147.568 1.00 55.58	C
ATOM	2081 CD2 LEU B 327		
	2082 N TYR B 328		N
		51.514 50.508 143.229 1.00 62.26	
		51.076 49.047 143.140 1.00 63.10	C
ATOM	2085 CD TVD D 228	50.702 48.523 144.172 1.00 62.38	0
ATOM	2000 CB TIRB 320	52.998 50.527 143.560 1.00 63.28 53.619 51.884 143.281 1.00 64.36	C C
ATOM	2087 CO TTR B 328	53.626 52.866 144.259 1.00 64.71	C
	2089 CD2 TYR B 328	54.168 52.171 142.050 1.00 64.48	C
	2090 CE1 TYR B 328	54.182 54.104 144.018 1.00 65.70	č
	2091 CE2 TYR B 328	54.716 53.413 141.810 1.00 65.61	Č
ATOM	2092 CZ TYR B 328	54.728 54.375 142.788 1.00 66.10	C
ATOM	2093 OH TYR B 328	55.288 55.604 142.502 1.00 67.55	0
ATOM	2094 N SER B 329	51.102 48.465 141.959 1.00 65.42	N
	2095 CA SER B 329	50.677 47.083 141.860 1.00 67.55	С
	2096 C SER B 329	51.719 46.193 142.513 1.00 70.65	С
	2097 O SER B 329	52.883 46.548 142.456 1.00 71.72	0
	2098 CB SER B 329	50.548 46.669 140.404 1.00 66.96	C
	2099 OG SER B 329	50.526 45.240 140.433 1.00 67.55	0
	2100 N GLUB 330	51.326 45.087 143.091 1.00 75.08	N
	2101 CA GLUB 330 2102 C GLUB 330	52.235 44.145 143.719 1.00 79.78	C
ATOM	2102 C GLUB 330	53.117 43.539 142.618 1.00 81.27	С

ATOM 2105 CG GLU B 330 50.421 41.080 143.122 1.00 91.03 ATOM 2106 CD GLU B 330 49.425 40.611 143.749 1.00 91.90 0 ATOM 2107 OE1 GLU B 330 50.493 41.081 141.857 1.00 92.57 ATOM 2108 OE2 GLU B 330 0 51.253 36.811 132.549 1.00 86.18 N ATOM 2109 N PHE B 337 ATOM 2110 CA PHE B 337 49.852 37.145 132.479 1.00 85.96 C ATOM 2111 C PHE B 337 48.997 36.001 131.933 1.00 85.36 C ATOM 2112 O PHE B 337 49.190 35.478 130.827 1.00 86.63 O 49.503 38.328 131.558 1.00 87.52 C ATOM 2113 CB PHE B 337 49.859 39.641 132.182 1.00 89.57 C ATOM 2114 CG PHE B 337 ATOM 2115 CD1 PHE B 337 49.843 39.761 133.566 1.00 90.51 C C 50.215 40.745 131.415 1.00 90.05 ATOM 2116 CD2 PHE B 337 C ATOM 2117 CE1 PHE B 337 50.181 40.970 134.162 1.00 91.28 C 50.547 41.952 132.014 1.00 90.08 ATOM 2118 CE2 PHE B 337 C ATOM 2119 CZ PHE B 337 50.530 42.072 133.389 1.00 90.52 ATOM 2120 N SER B 338 48.024 35.667 132.756 1.00 82.82 N ATOM 2121 CA SER B 338 47.075 34.617 132.372 1.00 80.39 C ATOM 2122 C SER B 338 45.740 35.093 132.927 1.00 78.40 C ATOM 2123 O SER B 338 45.783 35.839 133.928 1.00 77.87 0 C 47.493 33.300 133.019 1.00 80.21 ATOM 2124 CB SER B 338 ATOM 2125 OG SER B 338 47.758 33.540 134.398 1.00 79.73 0 44.629 34.666 132.354 1.00 75.87 ATOM 2126 N GLUB 339 N ATOM 2127 CA GLU B 339 43.342 35.081 132.949 1.00 74.09 C 43.526 35.122 134.469 1.00 72.45 С ATOM 2128 C GLUB 339 0 ATOM 2129 O GLUB 339 43.440 36.205 135.065 1.00 72.49 42.301 34.079 132.505 1.00 74.26 C ATOM 2130 CB GLU B 339 ATOM 2131 CG GLU B 339 41.030 33.874 133.294 1.00 74.49 C 39.898 33.645 132.292 1.00 75.67 C ATOM 2132 CD GLU B 339 ATOM 2133 OE1 GLU B 339 39.740 34.445 131.339 1.00 75.56 0 39.164 32.644 132.444 1.00 76.73 0 ATOM 2134 OE2 GLU B 339 43.858 33.991 135.105 1.00 70.10 ATOM 2135 N ALA B 340 N ATOM 2136 CA ALA B 340 44.067 33.983 136.538 1.00 68.16 C ATOM 2137 C ALA B 340 45.121 34.958 137.043 1.00 67.65 0 ATOM 2138 O ALA B 340 44.825 35.704 137.990 1.00 67.91 C ATOM 2139 CB ALA B 340 44.424 32.585 136.991 1.00 67.98 46.321 34.993 136.474 1.00 66.66 N ATOM 2140 N SER B 341 47.329 35.924 136.982 1.00 65.93 C ATOM 2141 CA SER B 341

46.854 37.355 136.798 1.00 65.12

47.080 38.127 137.749 1.00 65.86

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ATOM 2142 C SER B 341

ATOM 2143 O SER B 341

ATOM 2144 CB SER B 341

ATOM 2145 OG SER B 341

ATOM 2146 N MET B 342

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ATOM	2148 C MET B 342	44.654 39.478 136.444 1.00 60.47	С
ATOM	2149 O MET B 342	44.752 40.481 137.159 1.00 60.54	0
ATOM	2150 CB MET B 342	45.270 39.454 134.093 1.00 61.38	С
ATOM	2151 CG MET B 342	45.270 39.454 134.093 1.00 61.38 45.272 40.980 134.038 1.00 62.54	С
ATOM	2152 SD MET B 342	45.488 41.560 132.349 1.00 66.23	S
	2153 CE MET B 342		
	2154 N MET B 343	43.602 38.664 136.486 1.00 58.53	N
	2155 CA MET B 343	42.495 38.932 137.396 1.00 57.10	С
	2156 C MET B 343		С
	2157 O MET B 343		0
		41.513 37.780 137.393 1.00 56.26	C
ATOM	2159 CG MET B 343	40.589 37.839 136.195 1.00 56.11	С
		39.684 39.386 136.078 1.00 56.84	S
	2161 CE MET B 343		
	2162 N GLY B 344		N
	2163 CA GLY B 344	44.679 38.468 140.491 1.00 54.71	C
	2164 C GLY B 344	45.227 39.869 140.678 1.00 53.89	C
	2165 O GLY B 344		0
	2166 N LEUB 345		N
		46.621 41.760 140.042 1.00 54.09	C
		45.532 42.824 140.167 1.00 53.00	C
		45.490 43.579 141.140 1.00 53.38	0
		47.408 42.284 138.844 1.00 55.45	C
		48.757 41.626 138.559 1.00 57.40	C
	2172 CD1 LEU B 345 2173 CD2 LEU B 345		C C
ATOM ATOM			
	2175 CA LEU B 346	44.701 42.843 139.117 1.00 50.42 43.595 43.791 139.045 1.00 48.04	N
	2176 C LEU B 346		C C
		42.509 44.746 141.008 1.00 46.14	0
ATOM		42.828 43.449 137.782 1.00 47.72	C
	2179 CG LEU B 346	43.598 43.886 136.509 1.00 48.42	C
	2180 CD1 LEU B 346	42.660 43.796 135.311 1.00 48.05	C
	2181 CD2 LEU B 346	44.224 45.266 136.613 1.00 47.09	Č
	2182 N THR B 347	42.349 42.553 140.628 1.00 46.25	N
	2183 CA THR B 347	41.549 42.288 141.820 1.00 46.10	C
	2184 C THR B 347	42.238 42.666 143.100 1.00 47.12	c
	2185 O THR B 347	41.675 43.312 144.002 1.00 47.76	Ö
	2186 CB THR B 347	41.162 40.813 141.668 1.00 45.79	C
	2187 OG1 THR B 347	39.731 40.798 141.443 1.00 47.18	O
	2188 CG2 THR B 347	41.638 39.936 142.757 1.00 44.47	č
ATOM		43.516 42.349 143.245 1.00 48.37	N
	2190 CA ASN B 348	44.312 42.696 144.422 1.00 47.96	C
	2191 C ASN B 348	44.383 44.213 144.550 1.00 46.69	c
	2192 O ASN B 348	44.120 44.863 145.568 1.00 46.53	Ō

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ATOM	2193	CB ASN B 348	45.687 42.077 144.255 1.00 50.12	С
ATOM	2194	CG ASN B 348	46.646 42.472 145.355 1.00 53.52	С
ATOM	2195	OD1 ASN B 348	47.392 43.475 145.293 1.00 55.04	Ο
ATOM	2196	ND2 ASN B 348	46.576 41.621 146.382 1.00 54.64	N
ATOM	2197	N LEU B 349	44.729 44.861 143.440 1.00 45.19	N
ATOM	2198	CA LEU B 349	44.827 46.327 143.461 1.00 44.31	С
ATOM	2199	C LEU B 349	43.516 46.920 143.946 1.00 42.73	С
ATOM	2200	O LEU B 349	43,496 47,803 144,782 1,00 41,58	0
ATOM	2201	CB LEU B 349	45.260 46.806 142.070 1.00 44.84	С
ATOM	2202	CG LEU B 349	45.463 48.314 141.897 1.00 45.41	С
ATOM	2203	CD1 LEU B 349	46.548 48.802 142.850 1.00 45.52	С
ATOM	2204	CD2 LEU B 349	45.780 48.735 140.467 1.00 44.75	С
ATOM	2205	N ALA B 350	42.387 46.437 143.433 1.00 42.61	N
ATOM	2206	CA ALA B 350	41.064 46.936 143.776 1.00 42.37	С
ATOM	2207	C ALA B 350	40.836 46.794 145.268 1.00 42.95	С
ATOM	2208	O ALA B 350	40.543 47.737 146.002 1.00 41.96	O
ATOM	2209	CB ALA B 350	39.967 46.201 143.010 1.00 41.65	С
ATOM	2210	N ASP B 351	41.030 45.560 145.745 1.00 44.56	Ν
ATOM	2211	CA ASP B 351	40.862 45.330 147.181 1.00 46.40	С
ATOM	2212	C ASP B 351	41.664 46.319 148.016 1.00 46.43	С
ATOM	2213	O ASP B 351	41.230 46.750 149.090 1.00 47.39	Ο
ATOM	2214	CB ASP B 351	41.238 43.886 147.491 1.00 48.98	С
ATOM		CG ASP B 351	41.021 43.624 148.973 1.00 51.85	С
ATOM		OD1 ASP B 351	39.868 43.494 149.431 1.00 52.63	0
ATOM		OD2 ASP B 351	42.069 43.568 149.663 1.00 54.48	О
ATOM	2218	N ARG B 352	42.857 46.724 147.596 1.00 46.00	N
ATOM	2219	CA ARG B 352	43.654 47.672 148.350 1.00 45.92	С
ATOM		C ARG B 352	43.139 49.091 148.289 1.00 45.41	С
ATOM	2221	O ARG B 352	43.092 49.793 149.312 1.00 46.29	0
ATOM		CB ARG B 352	45.081 47.581 147.832 1.00 46.64	C
ATOM		CG ARG B 352	45.757 46.326 148.369 1.00 48.12	C
ATOM			47.240 46.699 148.620 1.00 49.94	С
ATOM		NE ARG B 352	47.831 46.493 147.298 1.00 52.10	N
		CZ ARG B 352	48.655 47.337 146.661 1.00 52.15	C
		NH1 ARG B 352	49.011 48.472 147.259 1.00 50.48	N
		NH2 ARG B 352	49.015 46.878 145.451 1.00 51.51	N
		N GLU B 353	42.701 49.536 147.119 1.00 44.33	N
		CA GLU B 353	42.161 50.889 146.991 1.00 43.49	C
ATOM		C GLU B 353	40.862 51.033 147.789 1.00 43.42	C
ATOM		O GLU B 353	40.503 52.128 148.220 1.00 42.92	0
		CB GLU B 353	41.848 51.196 145.537 1.00 42.87	C
		CG GLU B 353	42.933 50.836 144.558 1.00 43.52	C
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ATOM 2235 CD GLU B 353 42.710 51.456 143.201 1.00 44.16

ATOM 2236 OE1 GLU B 353 42.597 52.674 143.043 1.00 43.57

ATOM 2237 OE2 GLU B 353 42.628 50.706 142.214 1.00 45.84

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ATOM	2238	N LEU B 354	40.153 49.915 147.992 1.00 42.83	N
ATOM		CA LEUB 354	38.900 49.915 148.712 1.00 42.73	С
ATOM		C LEU B 354	39.083 50.455 150.110 1.00 43.31	С
		O LEU B 354	38.270 51.257 150.594 1.00 43.47	0
		CB LEUB 354	38.210 48.546 148.710 1.00 41.85	С
ATOM		CG LEUB 354	37.399 48.461 147.392 1.00 41.01	C
ATOM		CD1 LEUB 354	37.232 47.020 147.007 1.00 42.17	C
ATOM		CD2 LEUB 354	36.098 49.201 147.579 1.00 40.64	C
ATOM		N VAL B 355	40.192 50.012 150.697 1.00 43.66	N
ATOM		CA VALB 355	40.513 50.540 152.037 1.00 43.57	C
ATOM		C VAL B 355	40.640 52.049 151.989 1.00 43.49	C
ATOM		O VAL B 355	39.931 52.791 152.667 1.00 44.38	O C
ATOM		CB VAL B 355 CG1 VAL B 355	41.822 49.887 152.485 1.00 42.19 42.185 50.377 153.841 1.00 41.86	C
		CG2 VAL B 355	41.536 48.388 152.492 1.00 43.55	C
		N HIS B 356	41.502 52.573 151.138 1.00 43.64	N
ATOM		CA HIS B 356	41.663 54.020 151.046 1.00 44.98	C
ATOM		C HIS B 356	40.354 54.684 150.718 1.00 44.85	c
ATOM		O HIS B 356	40.075 55.789 151.171 1.00 44.94	Ö
ATOM		CB HIS B 356	42.746 54.342 150.000 1.00 48.00	C
ATOM		CG HIS B 356	44.039 53.806 150.549 1.00 50.79	C
ATOM		ND1 HIS B 356	44.987 54.578 151.156 1.00 51.64	N
ATOM	2260	CD2 HIS B 356	44.492 52.531 150.622 1.00 52.67	С
ATOM	2261	CE1 HIS B 356	45.975 53.804 151.555 1.00 52.82	С
ATOM	2262	NE2 HIS B 356	45.717 52.545 151.255 1.00 53.04	N
ATOM		N MET B 357	39.527 54.042 149.887 1.00 45.52	N
ATOM		CA MET B 357	38.258 54.585 149.440 1.00 43.50	С
ATOM		C MET B 357	37.366 54.938 150.612 1.00 43.20	C
ATOM			36.851 56.042 150.626 1.00 44.03	0
ATOM		CB MET B 357	37.424 53.666 148.547 1.00 42.56	C
ATOM		CG MET B 357	36.286 54.506 147.943 1.00 42.38	C
ATOM			35.245 53.437 146.919 1.00 43.60	S C
ATOM ATOM		CE MET B 357 N ILE B 358	36.318 53.100 145.547 1.00 42.88 37.213 53.978 151.513 1.00 42.20	N
ATOM		CA ILE B 358	36.378 54.184 152.687 1.00 42.20	C
ATOM		C ILEB 358	36.869 55.416 153.422 1.00 42.97	c
ATOM		O ILE B 358	36.054 56.284 153.754 1.00 43.92	Ö
ATOM		CB ILE B 358	36.483 52.950 153.581 1.00 39.18	C
ATOM		CG1 ILE B 358	35.909 51.759 152.836 1.00 39.34	Č
		CG2 ILE B 358	35.767 53.190 154.879 1.00 39.09	Č
		CD1 ILE B 358	36.019 50.424 153.527 1.00 39.80	č
		N ASN B 359	38.174 55.520 153.673 1.00 44.15	N
ATOM		CA ASN B 359	38,709 56,695 154,338 1.00 45.85	C
ATOM	2281		38.317 57.963 153.628 1.00 44.78	C
ATOM			37.738 58.868 154.190 1.00 45.76	0

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ATOM	2283	CB ASN B 359	40.230 56.589 154.376 1.00 50.87	С
		CG ASN B 359	40.498 55.579 155.477 1.00 56.26	С
		OD1 ASN B 359	40.076 55.925 156.602 1.00 61.30	Ο
		ND2 ASN B 359	41.104 54.423 155.259 1.00 57.59	N
		N TRP B 360	38.598 58.043 152.346 1.00 44.00	N
		CA TRP B 360	38.268 59.171 151.512 1.00 42.58	С
ATOM	2289	C TRP B 360	36.806 59.546 151.631 1.00 42.49	С
ATOM	2290	O TRP B 360	36.410 60.691 151.727 1.00 42.71	0
		CB TRP B 360	38.544 58.717 150.069 1.00 42.21	C
		CG TRP B 360	37.881 59.662 149.097 1.00 42.64	C
		CD1 TRP B 360	38.328 60.905 148.764 1.00 42.29	C
		CD2 TRP B 360	36.667 59.443 148.365 1.00 42.41	С
		NE1 TRP B 360	37.449 61.447 147.877 1.00 43.09	N
		CE2 TRP B 360	36.430 60.586 147.599 1.00 42.27	C
		CE3 TRP B 360	35.760 58.378 148.288 1.00 42.53	C
		CZ2 TRP B 360	35.342 60.733 146.752 1.00 42.40	C
		CZ3 TRP B 360	34.674 58.519 147.451 1.00 43.36	C C
		CH2 TRP B 360	34.462 59.688 146.688 1.00 43.36	N
		N ALA B 361	35.898 58.584 151.574 1.00 44.00	C
		CA ALA B 361	34.467 58.839 151.658 1.00 45.18	c
		C ALA B 361	34.177 59.629 152.930 1.00 46.34 33.398 60.572 152.903 1.00 45.79	0
		O ALA B 361	33.690 57.534 151.609 1.00 44.61	C
		CB ALA B 361 N LYS B 362	34.804 59.320 154.051 1.00 48.42	N ·
		CA LYS B 362	34.581 60.009 155.298 1.00 51.41	C
		C LYS B 362	34.844 61.494 155.237 1.00 51.60	c
		O LYS B 362	34.262 62.243 156.028 1.00 52.45	Ö
		CB LYS B 362	35.368 59.329 156.429 1.00 53.83	. C
		CG LYS B 362	34.783 57.948 156.761 1.00 56.54	С
		CD LYS B 362		С
		CE LYS B 362	33.243 57.135 158.619 1.00 60.68	С
		NZ LYS B 362	32.112 57.527 159.530 1.00 61.36	N
		N ARG B 363	35.659 61.990 154.354 1.00 51.98	N
ATOM	2316	CA ARG B 363	35.974 63.383 154.183 1.00 53.74	С
ATOM	2317	C ARG B 363	35.176 64.086 153.096 1.00 52.36	C
		O ARG B 363	35.421 65.265 152.810 1.00 53.34	0
		CB ARG B 363	37.445 63.546 153.759 1.00 57.28	C
		CG ARG B 363	38.196 62.254 153.990 1.00 63.66	C
		CD ARG B 363	38.649 62.308 155.471 1.00 69.44	C
		NE ARG B 363	39.675 63.365 155.438 1.00 74.98	N
		CZ ARG B 363	40.834 63.136 154.780 1.00 78.56	C
		NH1 ARG B 363	41.049 61.949 154.177 1.00 79.07	N
		NH2 ARG B 363	41.730 64.142 154.772 1.00 80.01	N
		N VAL B 364	34.268 63.458 152.393 1.00 50.64	N
ATOM	2327	CA VAL B 364	33.536 64.203 151.351 1.00 48.57	С

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ATOM	2328 C VAL B 364	32.516 64.992 152.132 1.00 48.30	С
ATOM	2329 O VAL B 364	31.679 64.424 152.834 1.00 49.68	0
ATOM	2330 CB VAL B 364	32.933 63.200 150.360 1.00 47.31	С
ATOM	2331 CG1 VAL B 364	31.906 63.840 149.457 1.00 46.60	С
ATOM	2332 CG2 VAL B 364	34.069 62.557 149.571 1.00 46.35	С
ATOM	2333 N PRO B 365	32.542 66.287 152.091 1.00 47.88	N
ATOM	2334 CA PRO B 365	31.625 67.148 152.817 1.00 47.75	С
ATOM	2335 C PRO B 365	30.208 66.645 152.701 1.00 47.86	С
ATOM	2336 O PRO B 365	29.722 66.392 151.609 1.00 48.96	0
ATOM	2337 CB PRO B 365	31.788 68.552 152.204 1.00 47.58	С
ATOM	2338 CG PRO B 365	33.260 68.466 151.902 1.00 49.17	С
ATOM	2339 CD PRO B 365	33.509 67.057 151.312 1.00 48.98	С
ATOM	2340 N GLY B 366	29.537 66.463 153.821 1.00 48.34	N
ATOM	2341 CA GLY B 366	28.168 66.023 153.933 1.00 48.09	C
ATOM	2342 C GLY B 366	27.949 64.535 154.121 1.00 47.88	С
ATOM	2343 O GLY B 366	26.864 64.089 154.545 1.00 48.29	0
ATOM	2344 N PHE B 367	28.970 63.754 153.775 1.00 46.58	N
ATOM	2345 CA PHE B 367	28.849 62.306 153.856 1.00 46.69	С
ATOM	2346 C PHE B 367	28.516 61.780 155.244 1.00 46.32	С
ATOM	2347 O PHE B 367	27.608 61.036 155.593 1.00 44.65	0
ATOM	2348 CB PHE B 367	30.145 61.654 153.357 1.00 45.74	С
ATOM	2349 CG PHE B 367	30.040 60.160 153.204 1.00 45.19	С
ATOM	2350 CD1 PHE B 367	29.373 59.598 152.150 1.00 44.90	С
ATOM	2351 CD2 PHE B 367	30.613 59.325 154.144 1.00 45.86	С
ATOM	2352 CE1 PHE B 367	29.287 58.234 152.008 1.00 46.05	С
ATOM	2353 CE2 PHE B 367	30.537 57.958 154.029 1.00 46.38	С
ATOM	2354 CZ PHE B 367	29.875 57.405 152.947 1.00 46.68	С
ATOM	2355 N VAL B 368	29.358 62.254 156.134 1.00 47.15	N
ATOM	2356 CA VAL B 368	29.376 61.923 157.550 1.00 48.33	С
ATOM	2357 C VAL B 368	28.103 62.324 158.245 1.00 49.61	С
ATOM	2358 O VAL B 368		0
ATOM	2359 CB VAL B 368	30.647 62.529 158.162 1.00 47.39	С
ATOM	2360 CG1 VAL B 368	30.341 63.282 159.413 1.00 47.29	C
ATOM	2361 CG2 VAL B 368	31.671 61.416 158.296 1.00 46.89	С
	2362 N ASP B 369	27.323 63.233 157.685 1.00 50.09	N
	2363 CA ASP B 369	26.035 63.587 158.254 1.00 50.46	С
ATOM	2364 C ASP B 369	25.034 62.476 157.971 1.00 48.55	C
ATOM		23.922 62.589 158.461 1.00 50.33	0
	2366 CB ASP B 369	25.475 64.892 157.668 1.00 53.89	C
	2367 CG ASP B 369	26.430 66.074 157.769 1.00 58.03	C
	2368 OD1 ASP B 369	27.112 66.330 158.802 1.00 59.26	0
	2369 OD2 ASP B 369	26.554 66.855 156.780 1.00 59.49	0
	2370 N LEUB 370	25.222 61.420 157.221 1.00 47.05	N
	2371 CA LEU B 370	24.202 60.401 156.985 1.00 45.34	C
ATOM	2372 C LEUB 370	24.280 59.335 158.062 1.00 43.86	С

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ATOM	2373	O LEUB 370		0
ATOM		CB LEU B 370		С
ATOM		CG LEU B 370	24.312 60.763 154.454 1.00 46.82	С
ATOM		CD1 LEU B 370	24.605 60.125 153.107 1.00 46.43	С
ATOM		CD2 LEU B 370	22.869 61.283 154.518 1.00 46.50	С
ATOM		N THR B 371	23.292 58.494 158.263 1.00 41.90	N
ATOM		CA THR B 371	23.420 57.495 159.308 1.00 42.13	С
ATOM		C THR B 371	24,521 56,534 158,912 1.00 43.67	С
ATOM		O THR B 371	24.823 56.337 157.727 1.00 44.74	0
ATOM		CB THR B 371	22.120 56.701 159.395 1.00 42.81	С
ATOM		OG1 THR B 371	21.749 56.371 158.054 1.00 44.14	О
ATOM	2384	CG2 THR B 371	20.990 57.552 159.918 1.00 43.46	С
ATOM	2385	N LEUB 372	25.132 55.886 159.899 1.00 44.52	N
ATOM	2386	CA LEU B 372	26.204 54.944 159.612 1.00 44.27	С
ATOM	2387	C LEU B 372	25.785 53.935 158.562 1.00 45.75	С
ATOM	2388	O LEUB 372	26,637 53,676 157,691 1.00 46.87	Ο
ATOM	2389	CB LEUB 372	26.618 54.282 160.915 1.00 43.07	С
ATOM	2390	CG LEU B 372	27.311 55.225 161.889 1.00 42.80	C
ATOM	2391	CD1 LEU B 372	27.664 54.482 163.168 1.00 43.31	C
ATOM		CD2 LEU B 372	28.594 55.751 161.277 1.00 43.66	С
ATOM		N HISB 373	24.566 53.395 158.585 1.00 45.98	N
ATOM		CA HISB 373	24.203 52.417 157.564 1.00 47.04	C
ATOM		C HIS B 373	24.055 53.084 156.212 1.00 46.53	C
ATOM		O HIS B 373	24.487 52.447 155.220 1.00 47.00	0
ATOM		CB HISB 373	23.005 51.585 157.954 1.00 49.76	C
ATOM		CG HISB 373	23.350 50.587 159.002 1.00 53.39	C
ATOM		ND1 HIS B 373	23.065 50.720 160.354 1.00 55.19	N
		CD2 HIS B 373	23.978 49.400 158.890 1.00 54.94	C
		CE1 HIS B 373	23.503 49.646 161.009 1.00 55.80	C
		NE2 HIS B 373	24.083 48.817 160.140 1.00 56.63	N N
		N ASP B 374	23.537 54.308 156.149 1.00 44.27	C
		CA ASP B 374	23.478 54.919 154.815 1.00 44.35 24.846 55.118 154.197 1.00 43.97	C
		C ASP B 374		Ö
		O ASP B 374		C
		CB ASP B 374 CG ASP B 374	21.223 55.703 155.009 1.00 48.08	Č
		OD1 ASP B 374	21.024 54.468 154.829 1.00 49.35	o
		OD2 ASP B 374	20.292 56.479 155.299 1.00 49.88	ő
		N GLN B 375	25.862 55.435 155.001 1.00 43.23	N
		CA GLN B 375	27.195 55.584 154.434 1.00 43.62	C
		C GLN B 375	27.589 54.230 153.874 1.00 44.32	C
ATOM			27.950 54.150 152.690 1.00 46.72	Ō
		CB GLN B 375	28.180 56.051 155.476 1.00 44.31	C
		CG GLN B 375	27.735 57.373 156.082 1.00 46.41	Č
		CD GLN B 375	28.564 57.807 157.274 1.00 46.26	С
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			0
ATOM	2418 OE1 GLN B 375	29.742 57.477 157.379 1.00 47.15	O N
		27.931 58.543 158.158 1.00 45.51 27.483 53.136 154.625 1.00 42.98	N
ATOM	2420 N VAL B 376	27.843 51.849 154.027 1.00 42.65	
ATOM	2421 CA VALB 376	27.054 51.662 152.740 1.00 43.08	c
ATOM	2422 C VAL B 376	27.611 51.284 151.714 1.00 43.58	Ŏ
		27.640 50.677 154.989 1.00 42.62	C
		28.412 49.481 154.467 1.00 42.57	C
		28.137 51.017 156.375 1.00 41.75	C
		25.753 51.934 152.711 1.00 44.02	N
		24.981 51.805 151.468 1.00 44.64	С
ATOM	2429 C HIS B 377	25.600 52.635 150.364 1.00 43.12	С
ATOM	2430 O HIS B 377	26.019 51.995 149.384 1.00 43.78	0
ATOM	2431 CB HIS B 377	23.497 52.076 151.711 1.00 46.21	С
ATOM	2432 CG AHIS B 377	22.607 52.039 150.512 0.50 44.35	С
		22.947 50.949 152.558 0.50 50.29	
ATOM	2434 ND1AHIS B 377	22.247 50.853 149.916 0.50 43.89	N
ATOM	2435 ND1BHIS B 377	22.350 51.163 153.793 0.50 51.12	N
ATOM	2436 CD2AHIS B 377	22.003 53.020 149.793 0.50 44.38 22.919 49.600 152.345 0.50 51.17	С
ATOM	2437 CD2BHIS B 377	22.919 49.600 152.345 0.50 51.17	C
		21.466 51.118 148.877 0.50 43.90	
		21.965 50.003 154.308 0.50 51.18 21.304 52.423 148.768 0.50 43.73	
ATOM	2440 NE2AIII3 D 377	22.299 49.039 153.458 0.50 51.65	N
ATOM	2441 NEZDIIIS D 377	25.768 53.948 150.396 1.00 41.23	N
		26.408 54.598 149.239 1.00 40.29	Ċ
		27.727 53.934 148.847 1.00 39.27	c
		28.095 53.717 147.675 1.00 37.62	Ō
ATOM	2446 CB LEUB 378	26.539 56.096 149.487 1.00 40.75	C
ATOM	2447 CG LEUB 378	25.290 56.820 149.987 1.00 40.78	С
ATOM	2448 CD1 LEU B 378	25.562 58.302 150.166 1.00 40.54	С
ATOM	2449 CD2 LEU B 378	24.139 56.634 149.024 1.00 40.52	С
ATOM	2450 N LEUB 379	28.540 53.551 149.829 1.00 38.80	N
	2451 CA LEUB 379	29.812 52.924 149.510 1.00 38.53	С
	2452 C LEUB 379	29.569 51.668 148.715 1.00 39.41	C
	2453 O LEUB 379	30.062 51.582 147.601 1.00 39.29	0
	2454 CB LEUB 379	30.626 52.631 150.754 1.00 37.75	C
	2455 CG LEUB 379	31.544 53.840 151.017 1.00 38.48	C
	2456 CD1 LEUB 379	32.100 53.599 152.411 1.00 40.54	C
	2457 CD2 LEU B 379	32.609 54.029 149.951 1.00 36.12	C
	2458 N GLUB 380	28.775 50.744 149.280 1.00 40.40	N C
	2459 CA GLUB 380	28.481 49.507 148.576 1.00 40.60 27.932 49.823 147.180 1.00 42.38	C
	2460 C GLU B 380 2461 O GLU B 380	28.273 49.192 146.186 1.00 41.89	0
	2462 CB GLUB 380	27.496 48.721 149.377 1.00 39.04	C
AIOM	*407 CD OPO D 300	21.470 40.121 147.511 1.00 57.04	

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ATOM	2463 CG	GLU B 380	28.010 48.175 150.668 1.00 43.02	С
ATOM		GLU B 380	26.849 47.489 151.386 1.00 46.45	С
ATOM		1 GLU B 380	25.689 47.970 151.219 1.00 48.79	0
ATOM	2466 OE	2 GLU B 380	27.057 46.480 152.108 1.00 47.08	0
ATOM		CYS B 381	27.068 50.823 147.051 1.00 44.02	N
ATOM	2468 CA	CYS B 381	26.504 51.108 145.760 1.00 46.42	С
ATOM	2469 C	CYS B 381	27.499 51.631 144.755 1.00 44.27	С
ATOM	2470 O	CYS B 381	27.485 51.113 143.630 1.00 42.52	0
ATOM	2471 CB	CYS B 381	25.216 51.950 145.913 1.00 50.98	С
ATOM	2472 SG	CYS B 381	23.759 50.890 145.506 1.00 62.03	S
ATOM	2473 N	ALA B 382	28.335 52.615 145.072 1.00 42.25	N
ATOM	2474 CA	ALA B 382	29.254 53.184 144.104 1.00 39.67	С
ATOM	2475 C	ALA B 382	30.697 52.743 144.082 1.00 39.72	С
ATOM	2476 O	ALA B 382	31.482 53.339 143.340 1.00 39.67	0
ATOM	2477 CB	ALA B 382	29.325 54.671 144.482 1.00 38.16	С
ATOM	2478 N	TRP B 383	31.121 51.713 144.797 1.00 39.88	N
ATOM		TRP B 383	32.543 51.357 144.827 1.00 39.09	С
ATOM		TRP B 383	33.224 51.210 143.495 1.00 39.22	C
ATOM		TRP B 383	34.192 51.900 143.161 1.00 39.38	0
ATOM		TRP B 383	32.724 50.169 145.722 1.00 38.40	С
ATOM	_	TRP B 383	32.290 48.861 145.180 1.00 37.57	C
ATOM			31.075 48.274 145.280 1.00 37.22	C
ATOM		2 TRP B 383	33.137 47.963 144.457 1.00 37.68	C
ATOM		1 TRP B 383	31.107 47.058 144.650 1.00 37.31	N C
ATOM		2 TRP B 383	32.354 46.839 144.130 1.00 37.64	C
ATOM		3 TRP B 383	34.470 48.015 144.037 1.00 37.73	C
ATOM	_	2 TRP B 383	32.871 45.765 143.407 1.00 37.19 34.977 46.951 143.322 1.00 37.29	C
ATOM	_	3 TRP B 383 2 TRP B 383	34.176 45.848 143.018 1.00 37.25	C
ATOM		LEU B 384	32.696 50.331 142.654 1.00 39.35	N
ATOM		LEU B 384	33,261 50.123 141.319 1.00 36.53	C
ATOM	_	LEU B 384		c
		LEU B 384	34.014 51.594 139.658 1.00 35.72	Ö
		LEU B 384	32.663 48.874 140.721 1.00 35.23	C
		LEU B 384	33.253 48.454 139.396 1.00 36.60	Č
		1 LEU B 384	34.772 48.345 139.412 1.00 36.92	C
		2 LEU B 384	32.657 47.092 139.012 1.00 37.73	Ċ
		GLU B 385	32.061 52.175 140.590 1.00 36.92	N
		GLU B 385	31.952 53.382 139.753 1.00 37.16	С
		GLU B 385	33.129 54.283 140.148 1.00 36.25	С
		GLU B 385	33.795 54.750 139.236 1.00 34.66	0
		GLU B 385	30.637 54.128 139.876 1.00 37.88	С
		GLU B 385	29.493 53.756 138.966 1.00 39.57	С
		GLU B 385	28.199 54.483 139.316 1.00 42.23	С
		1 GLU B 385	27.562 54.059 140.332 1.00 42.16	0
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ATOM	2508	OE2 GLU B 385	27.782 55.465 138.609 1.00 43.69	0
			33.352 54.447 141.461 1.00 36.36	N
			34.451 55.261 141.945 1.00 37.19	С
		C ILE B 386		С
		O ILE B 386		0
			34.645 55.361 143.455 1.00 37.43	С
			33.382 55.630 144.240 1.00 39.88	С
ATOM	2515	CG2 ILE B 386	35.634 56.462 143.765 1.00 36.99	С
ATOM	2516	CD1 ILE B 386	32.672 56.921 143.933 1.00 41.15	С
ATOM	2517	N LEUB 387	36.060 53.423 141.602 1.00 37.58	N
ATOM	2518	CA LEUB 387	37.306 52.866 141.102 1.00 38.24	С
ATOM		C LEUB 387		С
ATOM			38.582 53.432 139.162 1.00 40.64	О
ATOM	2521	CB LEU B 387	37.438 51.357 141.255 1.00 38.20	С
			37.692 50.790 142.649 1.00 38.34	С
			37.643 49.271 142.608 1.00 37.67	С
			39.021 51.311 143.173 1.00 38.66	С
ATOM	2525	N MET B 388	36.405 52.962 138.815 1.00 39.11	N
ATOM	2526	CA MET B 388		С
ATOM	2527	C MET B 388		С
ATOM		_	37.600 54.815 136.167 1.00 37.91	О
			35.309 52.641 136.601 1.00 37.03	С
			34.931 51.198 136.866 1.00 37.83	С
ATOM	2531	SD MET B 388	33.953 50.509 135.536 1.00 40.19	S
ATOM	2532	CE MET B 388		С
		N ILE B 389		N
			36.407 56.973 137.194 1.00 39.99	С
			37.852 57.311 137.529 1.00 41.00	C
			38.556 58.002 136.800 1.00 41.50	0
			35.399 57.998 137.723 1.00 38.80	C
			35.616 59.387 137.127 1.00 38.04	C
			35.499 58.074 139.230 1.00 38.43	C
			34.371 60.249 137.198 1.00 37.00	C
			38.360 56.778 138.629 1.00 41.85	N
		CA GLY B 390	39.739 57.039 139.007 1.00 43.61	C
		C GLY B 390	40.671 56.515 137.914 1.00 44.49	C
ATOM			41.563 57.248 137.453 1.00 44.84	0
		N LEUB 391	40.437 55.247 137.542 1.00 43.58	N
		CA LEUB 391	41.278 54.649 136.503 1.00 42.72	C
		C LEU B 391	41.281 55.524 135.266 1.00 43.00	C
		O LEU B 391	42.277 55.979 134.733 1.00 42.87	0
		CB LEUB 391	40.739 53.275 136.131 1.00 42.28	C
		CG LEUB 391	41.364 52.583 134.924 1.00 42.42	C
		CD1 LEU B 391	42.857 52.420 135.123 1.00 42.93	C
ATOM	2552	CD2 LEU B 391	40.780 51.204 134.661 1.00 42.70	С

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ATOM	2553 N VAL B 392	40.083 55.797 134.767 1.00 44.30	N
ATOM		39.888 56.599 133.564 1.00 44.62	С
ATOM		40.696 57.890 133.661 1.00 45.80	С
ATOM		41.483 58.277 132.782 1.00 46.09	0
	2557 CB VAL B 392	38,385 56,870 133,329 1.00 42.95	С
	2558 CG1 VAL B 392	38.164 57.928 132.274 1.00 42.03	С
	2559 CG2 VAL B 392	37,697 55,589 132,880 1.00 41.82	С
	2560 N TRP B 393	40.489 58.565 134.786 1.00 46.23	N
	2561 CA TRP B 393	41.156 59.836 135.033 1.00 47.70	С
	2562 C TRP B 393	42.668 59.730 135.000 1.00 48.44	С
ATOM		43.349 60.532 134.370 1.00 50.15	0
	2564 CB TRP B 393	40.728 60.368 136.388 1.00 47.66	С
	2565 CG TRP B 393	– .	C
	2566 CD1 TRP B 393	42.529 61.268 137.963 1.00 49.10	С
	2567 CD2 TRP B 393	41.793 62.749 136.452 1.00 49.37	С
	2568 NE1 TRP B 393	43.196 62.453 138.162 1.00 48.69	N
	2569 CE2 TRP B 393	42.762 63.374 137.260 1.00 48.40	С
	2570 CE3 TRP B 393	41.179 63.478 135.425 1.00 49.82	С
	2571 CZ2 TRP B 393	43.122 64.691 137.078 1.00 48.39	С
	2572 CZ3 TRP B 393	41.546 64.799 135.246 1.00 49.75	С
	2573 CH2 TRP B 393	42.503 65.383 136.081 1.00 49.28	С
	2574 N ARG B 394	43.221 58.741 135.690 1.00 48.15	N
	2575 CA ARG B 394	44.665 58.624 135.677 1.00 48.22	С
	2576 C ARG B 394	45.114 58.067 134.345 1.00 49.34	С
	2577 O ARG B 394	46.307 58.107 134.051 1.00 50.97	Ο
ATOM	2578 CB ARG B 394	45.277 57.829 136.820 1.00 47.90	С
ATOM	2579 CG ARG B 394	44.677 56.582 137.366 1.00 46.59	С
ATOM	2580 CD ARG B 394	45.468 56.021 138.547 1.00 45.18	С
ATOM	2581 NE ARG B 394	45.074 54.602 138.668 1.00 46.07	N
ATOM	2582 CZ ARG B 394	43.930 54.222 139.261 1.00 46.64	С
ATOM	2583 NH1 ARG B 394	43.142 55.189 139.769 1.00 46.63	N
ATOM	2584 NH2 ARG B 394	43.605 52.934 139.334 1.00 45.08	N
ATOM	2585 N SER B 395	44.231 57.530 133.519 1.00 50.71	N
ATOM	2586 CA SER B 395	44.647 56.956 132.249 1.00 51.33	С
ATOM	2587 C SER B 395	44.612 57.948 131.116 1.00 53.69	C _i
ATOM	2588 O SER B 395	45.009 57.595 130.014 1.00 52.96	О
ATOM	2589 CB SER B 395	43.671 55.822 131.926 1.00 50.07	С
ATOM	2590 OG SER B 395	44.140 54.648 132.551 1.00 50.14	О
ATOM	2591 N MET B 396	44.095 59.141 131.377 1.00 57.28	N
	2592 CA MET B 396	43.935 60.187 130.401 1.00 60.41	С
	2593 C MET B 396	45.075 60.457 129.431 1.00 63.46	С
	2594 O MET B 396	44.857 60.432 128.205 1.00 63.38	0
	2595 CB MET B 396	43.710 61.506 131.146 1.00 60.26	С
	2596 CG MET B 396	42.519 62.275 130.599 1.00 61.44	С
ATOM	2597 SD MET B 396	41.916 63.340 131.936 1.00 63.26	S

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	2598 CE MET B 396	42.092 64.928 131.150 1.00 63.32	C
		46.269 60.729 129.980 1.00 65.76	N
ATOM		47.405 61.033 129.138 1.00 68.66	С
ATOM		48.127 59.824 128.639 1.00 67.15	С
ATOM		49.341 59.857 128.451 1.00 68.54	0
ATOM		48.455 61.883 129.846 1.00 74.19	C
ATOM	2604 CG GLUB 397	47.902 63.090 130.581 1.00 81.83	С
ATOM	2605 CD GLUB 397	47.274 62.607 131.891 1.00 86.58 47.662 61.462 132.279 1.00 87.97	С
ATOM	2606 OE1 GLUB 397	47.662 61.462 132.279 1.00 87.97	0
ATOM		46.420 63.332 132.488 1.00 89.52	0
		47.570 58.658 128.443 1.00 65.63	N
ATOM		48.211 57.461 127.941 1.00 64.09	С
ATOM	2610 C HIS B 398	47.197 56.851 126.970 1.00 62.84	С
ATOM	2611 O HIS B 398		0
ATOM		48.584 56.429 128.983 1.00 65.04	С
		49.573 56.912 129.992 1.00 66.53	С
		49.334 58.079 130.682 1.00 67.12	N
ATOM		50.750 56.456 130.455 1.00 67.25	С
ATOM		50.288 58.363 131.527 1.00 68.05	С
ATOM		51.161 57.376 131.402 1.00 68.83	N
		46.994 57.547 125.863 1.00 61.30	N
	2619 CA PRO B 399		С
ATOM	2620 C PRO B 399		С
ATOM			0
ATOM	2622 CB PRO B 399		C
ATOM		47.011 59.217 124.246 1.00 60.94	C
ATOM		47.706 58.775 125.500 1.00 60.85	C
ATOM			N
ATOM	2626 CA GLY B 400		С
ATOM		45.542 52.704 125.217 1.00 57.83	C
ATOM		45.492 51.471 125.033 1.00 58.86	0
	2629 N LYS B 401	45.915 53.242 126.369 1.00 56.30	N
	2630 CA LYS B 401	46.304 52.433 127.494 1.00 55.69	C
	2631 C LYS B 401	45.550 52.773 128.782 1.00 53.97	C
	2632 O LYS B 401	44.950 53.834 128.945 1.00 53.24	0
	2633 CB LYS B 401	47.760 52.670 127.822 1.00 58.12	C
	2634 CG LYS B 401	48.775 52.737 126.722 1.00 61.08	C
	2635 CD LYS B 401	49.742 51.563 126.877 1.00 64.21	C
	2636 CE LYS B 401	50.482 51.307 125.564 1.00 66.02	C
	2637 NZ LYS B 401	51.024 52.633 125.124 1.00 67.99	N
ATOM		45.640 51.805 129.691 1.00 51.90	N
	2639 CA LEUB 402	45.012 51.988 130.990 1.00 51.47	С
	2640 C LEUB 402	46.091 51.851 132.079 1.00 51.01	C
	2641 O LEUB 402	46.703 50.795 132.242 1.00 50.99	0
ATOM	2642 CB LEUB 402	43.866 51.034 131.283 1.00 50.72	С

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ATOM	2643	CG LEUB 402	42.665 51.047 130.345 1.00 50.65	С
ATOM	2644	CD1 LEU B 402	41.818 49.791 130.586 1.00 51.08	С
ATOM	2645	CD2 LEU B 402	41.830 52.300 130.522 1.00 49.10	С
ATOM	2646	N LEU B 403	46.285 52.928 132.827 1.00 49.42	N
ATOM	2647	CA LEU B 403	47.230 52.971 133.906 1.00 48.91	С
ATOM	2648	C LEU B 403	46.653 52.489 135.221 1.00 48.89	С
ATOM	2649		46.344 53.335 136.081 1.00 49.61	0
ATOM	2650		47.635 54.452 134.090 1.00 50.09	С
ATOM	2651	CG LEUB 403	48.949 54.589 134.873 1.00 50.88	С
ATOM	2652	CD1 LEU B 403	50.141 54.474 133.943 1.00 50.73	С
ATOM	2653	CD2 LEU B 403	48.971 55.896 135.626 1.00 51.49	С
ATOM	2654	N PHE B 404	46.515 51.182 135.453 1.00 48.07	N
ATOM	2655	CA PHE B 404	45.970 50.750 136.745 1.00 48.28	С
ATOM	2656	C PHE B 404	46.818 51.327 137.861 1.00 49.45	С
ATOM	2657	O PHE B 404	46.299 51.826 138.854 1.00 50.59	0
ATOM	2658	CB PHE B 404	45.845 49.232 136.911 1.00 47.54	С
ATOM	2659	CG PHE B 404	44.705 48.761 136.042 1.00 47.17	С
ATOM	2660		44.918 48.494 134.696 1.00 47.57	С
			43.442 48.625 136.566 1.00 47.02	С
			43.881 48.078 133.880 1.00 47.18	C
		_	42.401 48.207 135.759 1.00 47.59	C
		CZ PHE B 404	42.619 47.926 134.415 1.00 47.23	С
		N ALA B 405	48.123 51.241 137.700 1.00 51.22	N
		CA ALA B 405	49.104 51.761 138.632 1.00 53.22	С
		C ALA B 405	50.194 52.524 137.898 1.00 54.37	C
		O ALA B 405	50.376 52.443 136.687 1.00 55.44	0
		CB ALA B 405	49.744 50.597 139.382 1.00 52.66	C
		N PRO B 406	51.038 53.219 138.656 1.00 55.09	N
			52.179 53.966 138.148 1.00 54.47	C
ATOM	2672	C PRO B 406	53.075 52.904 137.526 1.00 54.12	С
ATOM	2673	O PRO B 406	53.693 53.198 136.519 1.00 56.78	0
			52.865 54.697 139.295 1.00 53.61	C
		CG PRO B 406	51.876 54.542 140.395 1.00 53.88	C
		CD PRO B 406	50.980 53.359 140.110 1.00 54.88	C
		N ASN B 407	53.112 51.726 138.094 1.00 52.81	N
		CA ASN B 407	53.875 50.628 137.605 1.00 53.06	С
		C ASN B 407	53.019 49.505 137.050 1.00 54.38	C
		O ASN B 407	53,463 48,349 137,090 1.00 55.05	0
		CB ASN B 407	54.750 50.056 138.697 1.00 54.10	C
		CG ASN B 407	53.941 49.244 139.687 1.00 55.16	C
		OD1 ASN B 407	52.821 49.611 140.031 1.00 56.90	O
		ND2 ASN B 407	54.492 48.136 140.145 1.00 55.04	N
		N LEUB 408	51.825 49.796 136.536 1.00 55.00	N C
		CA LEUB 408	51.037 48.720 135.898 1.00 55.25	C
ATOM	2687	C LEU B 408	50.281 49.440 134.782 1.00 55.80	C

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		1	0
ATOM	2688 O LEUB 408	49.300 50.096 135.101 1.00 56.45	0
		50.086 47.950 136.763 1.00 54.97	C C
		49.227 46.846 136.146 1.00 54.42	
	2691 CD1 LEU B 408	50.000 45.958 135.197 1.00 53.91	C
	2692 CD2 LEU B 408	48.622 45.981 137.252 1.00 53.90	C
	2693 N LEUB 409	50.773 49.331 133.557 1.00 56.16	N
		50.123 50.051 132.449 1.00 55.57	С
	2695 C LEUB 409		C
		50.456 48.791 130.491 1.00 58.54	0
ATOM	2697 CB LEU B 409	51.154 51.029 131.942 1.00 54.18	C
ATOM	2698 CG LEU B 409	50.964 51.930 130.767 1.00 54.11	С
		49.533 52.409 130.593 1.00 55.16	C
		51.811 53.184 130.983 1.00 55.61	C
ATOM			N
		48.040 47.576 130.462 1.00 56.51	С
ATOM	2703 C LEUB 410	47.654 48.400 129.236 1.00 58.67	C
		47.424 49.609 129.253 1.00 58.30	0
		46.927 46.648 130.931 1.00 54.31	C
ATOM		47.304 46.011 132.267 1.00 53.90	С
		46.197 45.127 132.803 1.00 54.71	C
ATOM	2708 CD2 LEU B 410	48.599 45.250 132.068 1.00 53.46	C
		47.623 47.657 128.154 1.00 61.24	N
		47.285 48.161 126.839 1.00 63.87	С
		46.009 47.463 126.404 1.00 63.71	С
ATOM		45.761 46.311 126.804 1.00 63.85	0
ATOM	2713 CB ASP B 411	48.535 47.803 126.035 1.00 68.46	C C
ATOM	2714 CG ASP B 411	48.223 47.528 124.579 1.00 72.49	
ATOM	2715 ODI ASP B 411	47.638 46.434 124.363 1.00 74.61	0
		48.538 48.418 123.742 1.00 74.14	O
ATOM		45.191 48.092 125.568 1.00 63.39	N C
		43.966 47.441 125.156 1.00 64.41	
	2719 C ARG B 412	44.074 45.937 124.950 1.00 65.37	C
	2720 O ARG B 412	43.387 45.129 125.574 1.00 64.97	0
	2721 CB ARG B 412	43.395 48.061 123.872 1.00 64.50	C
	2722 CG ARG B 412	42.348 47.114 123.280 1.00 64.68	C
	2723 CD ARG B 412	41.448 47.797 122.300 1.00 65.82	C
	2724 NE ARG B 412		N
	2725 CZ ARG B 412	40.212 45.855 121.425 1.00 66.51	C
	2726 NH1 ARG B 412	41.336 45.265 121.017 1.00 66.41	N
ATOM		39.024 45.297 121.244 1.00 66.53	N
	2728 N ASN B 413	44.934 45.502 124.043 1.00 67.17	N
	2729 CA ASN B 413	45.090 44.091 123.729 1.00 69.50	C
	2730 C ASN B 413	45.366 43.206 124.904 1.00 68.94	C
	2731 O ASN B 413	44.960 42.029 124.885 1.00 69.91	0
ATOM	2732 CB ASN B 413	46.169 43.941 122.641 1.00 73.00	С

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****	yd.20012	173/371	
ATOM	2823 CD2 PHE B 4	42.031 46.381 128.907 1.00 47.63	С
ATOM	2824 CE1 PHE B 4	25 40.983 45.815 131.396 1.00 47.70	С
ATOM	2825 CE2 PHE B 4	25 42.833 45.916 129.923 1.00 48.04	С
ATOM	2826 CZ PHE B 4	25 42.321 45.625 131.176 1.00 47.39	Ċ
ATOM	2827 N ASP B 42	6 37.448 48.532 126.499 1.00 49.87	N
ATOM	2828 CA ASP B 4	26 37.056 49.426 125.412 1.00 50.42	С
ATOM	2829 C ASP B 42	6 36.260 50.583 125.947 1.00 50.41	С
ATOM	2830 O ASP B 42	6 36.621 51.751 125.704 1.00 50.89	0
ATOM	2831 CB ASP B 4	26 36.416 48.590 124.331 1.00 53.00	С
ATOM	2832 CG ASP B 4	26 37,493 48,057 123,392 1.00 55.59	С
ATOM	2833 OD1 ASP B 4	38.621 48.596 123.480 1.00 56.98	О
ATOM	2834 OD2 ASP B 4	37.224 47.143 122.584 1.00 57.24	Ο
ATOM	2835 N MET B 4	35.223 50.294 126.740 1.00 49.36	N
ATOM	2836 CA MET B 4	27 34.406 51.361 127.343 1.00 47.10	C
ATOM	2837 C MET B 42	35.274 52.289 128.191 1.00 45.73	С
ATOM	2838 O MET B 43	27 35.167 53.530 128.150 1.00 43.48	О
ATOM	2839 CB MET B 4	33,310 50,689 128,159 1,00 47,07	С
ATOM	2840 CG MET B 4	32.326 49.996 127.228 1.00 48.35	С
ATOM	2841 SD MET B 4	27 30.954 49.295 128.150 1.00 51.41	S
ATOM	2842 CE MET B 4	27 31.695 47.858 128.915 1.00 50.08	
		8 36.196 51.637 128.952 1.00 43.54	N
ATOM	2844 CA LEUB 4	28 37.108 52.444 129.758 1.00 41.57	C
		8 37.918 53.393 128.895 1.00 42.27	C
ATOM	2846 O LEUB 42	8 37.993 54.612 129.123 1.00 41.21	0
ATOM	2847 CB LEUB 4	28 37.967 51.529 130.595 1.00 39.86	C
ATOM	2848 CG LEUB 4	28 37.222 50.863 131.757 1.00 39.33 428 38.136 49.799 132.341 1.00 39.15	C
ATOM	2849 CD1 LEU B	428 38.136 49.799 132.341 1.00 39.15	C
ATOM	2850 CD2 LEU B	428 36.829 51.864 132.828 1.00 38.57	C
ATOM	2851 N LEUB 42	9 38.515 52.861 127.811 1.00 43.16	N
ATOM	2852 CA LEUB 4	29 39.324 53.737 126.937 1.00 42.07	C
		9 38.533 54.891 126.369 1.00 41.89	
		9 38.920 56.061 126.439 1.00 40.64	O C
	2855 CB LEUB 4		C
	2856 CG LEUB 4		C .
	2857 CD1 LEUB		C
	2858 CD2 LEU B		N
	2859 N ALAB 43		C
	2860 CA ALAB		c
	2861 C ALAB 43		O .
	2862 O ALAB 43		C
	2863 CB ALAB 4 2864 N THR B 4		N
	2865 CA THR B 4		Ċ
	2866 C THR B 43		С
	2867 O THR B 43		Ŏ
AIOM	2001 O TIECD 4.	71 30,747 37,437 120,101 1,00 43,03	•

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4 TO 1 4	2040 CD TUD D 421	35.365 56.767 129.941 1.00 43.22	С
	2868 CB THR B 431	34,490 55,700 129,613 1.00 44.07	0
		34.770 57.811 130.856 1.00 42.46	Č
		38.036 57.451 128.885 1.00 45.42	N
ATOM	2872 CA SER B 432	39.336 58.071 129.093 1.00 46.40	C
		39.624 59.090 128.007 1.00 47.18	C
		40.081 60.200 128.226 1.00 46.93	0
ATOM	2875 CB SER B 432	40.426 57.005 129.165 1.00 46.68	C
ATOM	2876 OG SER B 432	41.615 57.762 129.362 1.00 47.93	0
		39.322 58.696 126.779 1.00 49.00	N
ATOM	2878 CA SER B 433	39.439 59.529 125.597 1.00 50.60	C
ATOM	2879 C SER B 433	38.550 60.765 125.663 1.00 51.04	С
ATOM	2880 O SER B 433	38.936 61.913 125.493 1.00 49.73	0
ATOM	2881 CB SER B 433	38.936 61.913 125.493 1.00 49.73 38.933 58.601 124.478 1.00 51.44	С
ATOM	2882 OG SER B 433	39.347 59.183 123.261 1.00 54.59	0
		37.257 60.564 125.992 1.00 52.57	N
		36.343 61.687 126.091 1.00 53.56	С
	2885 C ARG B 434		С
	2886 O ARG B 434		0
	2887 CB ARG B 434		C C
ATOM	2888 CG ARG B 434	34.002 62.475 126.553 1.00 57.09 32.656 62.443 125.853 1.00 59.84	
ATOM	2889 CD ARG D 434	31.929 63.746 125.929 1.00 62.03	N N
ATOM	2801 C7 ARGR 434	32.361 64.759 125.146 1.00 62.85	C
	2892 NH1 ARG B 434		
	2893 NH2 ARG B 434		N
	2894 N PHE B 435		N
ATOM	2895 CA PHE B 435	37.988 63.060 129.258 1.00 56.24	C
ATOM	2896 C PHE B 435	39.122 63.878 128.661 1.00 57.90	C
ATOM	2897 O PHE B 435	39.213 65.071 128.914 1.00 57.34	Ο
		38.418 62.337 130.527 1.00 56.05	С
ATOM	2899 CG PHE B 435	37.308 62.036 131.502 1.00 56.15	C
	2900 CD1 PHE B 435	36.024 62.524 131.369 1.00 55.57	С
	2901 CD2 PHE B 435	37.568 61.227 132.593 1.00 56.19	С
	2902 CE1 PHE B 435	35.037 62.232 132.264 1.00 55.28	С
	2903 CE2 PHE B 435	36.594 60.905 133.516 1.00 56.05	С
	2904 CZ PHE B 435	35.316 61.417 133.338 1.00 56.32	С
	2905 N ARG B 436	39.955 63.231 127.854 1.00 60.28	N
	2906 CA ARG B 436	41.058 63.905 127.192 1.00 62.39	C
	2907 C ARGB 436	40.479 65.002 126.321 1.00 63.40	C
	2908 O ARG B 436	40.774 66.177 126.463 1.00 64.03	O C
	2909 CB ARG B 436 2910 CG ARG B 436	41.829 62.929 126.314 1.00 63.83	C
	2911 CD ARG B 436	43.304 63.231 126.193 1.00 66.34 44.026 62.204 125.336 1.00 69.23	C
	2911 CD ARG B 436 2912 NE ARG B 436		N
ATOM	2912 NE ARG B 430	43.917 00.630 123.633 1.00 /1.00	14

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ATOM	2958 CA GLY B 442	41.451 67.852 138.380 1.00 58.59	С
ATOM	2959 C GLY B 442	40.381 68.371 139.311 1.00 57.45	С
ATOM	2960 O GLY B 442	39.750 67.550 139.971 1.00 57.67	Ο
ATOM	2961 N GLUB 443	40.110 69.665 139.394 1.00 57.46	N
ATOM	2962 CA GLUB 443	39.071 70.172 140.290 1.00 58.76	С
ATOM	2963 C GLU B 443	37.701 69.598 139.853 1.00 56.56	C
ATOM	2964 O GLUB 443	36.801 69.336 140.659 1.00 55.98	0
ATOM	2965 CB GLUB 443	38.915 71.685 140.392 1.00 61.69	C
ATOM	2966 CG GLUB 443	40.077 72.578 140.705 1.00 65.54	C
ATOM	2967 CD GLUB 443	41.234 72.324 139.750 1.00 69.36	C
ATOM	2968 OE1 GLUB 443	41.018 72.218 138.513 1.00 70.43	0
ATOM		42.375 72.210 140.277 1.00 71.96 37.557 69.444 138.539 1.00 53.20	N
ATOM	2971 CA GLUB 444	36.342 68.887 137.981 1.00 50.57	C
ATOM	2972 C GLU B 444	36.286 67.415 138.361 1.00 49.12	c
	2973 O GLUB 444	35.270 66.955 138.881 1.00 49.11	Ö
	2974 CB GLU B 444	36.350 69.031 136.465 1.00 50.33	C
	2975 CG GLUB 444	35,989 70,466 136,085 1.00 49.89	Ċ
ATOM		36.187 70.701 134.602 1.00 50.08	С
ATOM	2977 OE1 GLU B 444	37.163 70.127 134.046 1.00 49.93	0
ATOM	2978 OE2 GLU B 444	35.324 71.458 134.107 1.00 50.00	Ο
ATOM	2979 N PHE B 445	37.398 66.720 138.123 1.00 47.04	N
ATOM		37.485 65.299 138.458 1.00 45.59	С
ATOM	2981 C PHE B 445	36.995 64.993 139.867 1.00 46.10	C
ATOM	2982 O PHE B 445	36.101 64.205 140.163 1.00 46.63	0
ATOM	2983 CB PHE B 445	38.919 64.814 138.315 1.00 43.27	C
ATOM		39.145 63.452 138.876 1.00 42.65	C C
ATOM		38.452 62.370 138.401 1.00 43.72 40.046 63.227 139.881 1.00 43.37	C
ATOM ATOM	2987 CE1 PHE B 445	38.644 61.098 138.909 1.00 44.67	Č
ATOM	2988 CE2 PHE B 445	40.284 61.979 140.419 1.00 43.66	Č
	2989 CZ PHE B 445	39.574 60.907 139.917 1.00 44.59	Č
	2990 N VAL B 446	37.590 65.656 140.833 1.00 46.31	N
	2991 CA VAL B 446	37.277 65.532 142.254 1.00 46.33	С
	2992 C VAL B 446	35.810 65.787 142.543 1.00 47.52	С
ATOM	2993 O VAL B 446	35.184 65.166 143.431 1.00 48.08	Ο
ATOM	2994 CB VAL B 446	38.311 66.442 142.934 1.00 45.14	С
	2995 CG1 VAL B 446	37.743 67.475 143.832 1.00 45.02	С
	2996 CG2 VAL B 446	39.302 65.572 143.699 1.00 45.97	С
	2997 N CYS B 447	35.158 66.685 141.809 1.00 47.38	N
	2998 CA CYS B 447	33.755 66.952 142.040 1.00 48.88	С
	2999 C CYS B 447	32.865 65.818 141.558 1.00 49.14	C
	3000 O CYS B 447	31.941 65.374 142.235 1.00 49.68	0
	3001 CB CYS B 447	33.375 68.225 141.275 1.00 50.13	C S
ATOM	3002 SG CYS B 447	33.720 69.719 142.194 1.00 53.53	3

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			177/371	
ATOM	3003	N LEUB 448	33.122 65.336 140.341 1.00 48.95	N
ATOM		CA LEU B 448	32.344 64.260 139.734 1.00 47.16	С
ATOM		C LEU B 448	32.437 63.023 140.618 1.00 46.56	С
ATOM		O LEUB 448	31.432 62.376 140.924 1.00 47.61	0
ATOM		CB LEU B 448	32.865 63.902 138.361 1.00 47.65	С
ATOM		CG LEUB 448	32.616 64.881 137.213 1.00 48.16	С
ATOM		CD1 LEU B 448	33.430 64.435 135.992 1.00 48.65	C
		CD2 LEU B 448	31.135 64.937 136.890 1.00 47.17	С
ATOM	3011	N LYS B 449	33.650 62.740 141.087 1.00 44.57	N
ATOM	3012	CA LYS B 449	33.830 61.590 141.963 1.00 43.44	С
ATOM		C LYS B 449	32.912 61.728 143.151 1.00 43.26	С
ATOM		O LYS B 449	32.262 60.740 143.539 1.00 44.55	0
		CB LYS B 449	35.304 61.464 142.272 1.00 44.12	C
		CG LYS B 449	35.798 60.032 142.426 1.00 44.36	C
		CD LYS B 449	36.782 60.041 143.569 1.00 45.90	C
		CE LYS B 449	38.197 60.360 143.103 1.00 46.74	C
		NZ LYS B 449	39.081 60.103 144.303 1.00 48.51	N
ATOM		N SER B 450	32.765 62.899 143.767 1.00 42.43	N C
		CA SER B 450	31.846 62.976 144.909 1.00 42.81 30.399 62.836 144.484 1.00 41.70	c
		C SER B 450	29.594 62.261 145.208 1.00 42.04	0
ATOM		O SER B 450 CB SER B 450	31.905 64.329 145.633 1.00 44.22	C
ATOM ATOM		OG SER B 450	33.285 64.483 145.953 1.00 48.34	Ö
ATOM		N ILE B 451	30.067 63.392 143.318 1.00 40.21	N
		CA ILE B 451	28.689 63.295 142.852 1.00 38.74	Ċ
		C ILE B 451	28.361 61.816 142.756 1.00 38.58	c
ATOM		O ILE B 451	27.305 61.378 143.211 1.00 37.33	Ö
ATOM		CB ILE B 451	28.571 64.007 141.514 1.00 39.81	С
			28.772 65.508 141.765 1.00 40.80	С
		CG2 ILE B 451	27,239 63.690 140.853 1.00 39.99	С
ATOM	3033	CD1 ILE B 451	28.421 66.370 140.544 1.00 42.17	·C
ATOM	3034	N ILE B 452	29.284 61.035 142.170 1.00 38.63	N
		CA ILE B 452	29.082 59.592 142.020 1.00 37.62	С
		C ILE B 452	28.825 58.938 143.373 1.00 38.09	C
		O ILE B 452	27.889 58.162 143.541 1.00 37.47	0
		CB ILE B 452	30.270 58.895 141.326 1.00 36.64	C
		CG1 ILE B 452	30.469 59.451 139.926 1.00 36.43	C
		CG2 ILE B 452	30.041 57.381 141.292 1.00 36.66	C
		CD1 ILE B 452	31.347 58.695 138.958 1.00 35.50	C
		N LEUB 453	29.658 59.254 144.362 1.00 38.77	N
		CA LEUB 453	29.499 58.683 145.683 1.00 39.54	C C
		C LEUB 453	28.130 59.031 146.243 1.00 40.27 27.508 58.168 146.829 1.00 41.50	0
		O LEUB 453	30.559 59.195 146.693 1.00 38.52	C
		CB LEU B 453 CG LEU B 453	30.359 39.193 146.693 1.00 38.32 30.293 58.818 148.163 1.00 36.48	C
AIUM	/ 44در	CG LEU B 433	JULES JOIOTO 170,1U3 1,UU JU.40	C

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ATOM 3083 N TYR B 459

ATOM 3084 CA TYR B 459

ATOM 3085 C TYR B 459

ATOM 3086 O TYR B 459

ATOM 3087 CB TYR B 459

ATOM 3088 CG TYR B 459

ATOM 3089 CD1 TYR B 459

ATOM 3090 CD2 TYR B 459

ATOM 3091 CE1 TYR B 459

ATOM 3092 CE2 TYR B 459

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SUBSTITUTE SHEET (RULE 26)

18.463 56.574 145.390 1.00 79.87

16.946 54.676 145.792 1.00 86.55

16.030 53.954 145.393 1.00 88.11

16.803 55.878 143.650 1.00 85.70

17.118 57.209 142.998 1.00 87.73

18.413 57.461 142.558 1.00 88.64

16.167 58.203 142.864 1.00 88.88

18.719 58.680 141.989 1.00 90.47

16.465 59.434 142.302 1.00 90.05

17.134 56.038 145.167 1.00 84.11

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		100/5/1	
ATOM	3141 CB SER B 468	14.518 57.369 153.865 1.00100.33	C
ATOM	3142 OG SER B 468	14.946 56.142 154.419 1.00101.36 13.669 60.334 154.008 1.00 92.58	0
ATOM	3143 N LEUB 469	13.669 60.334 154.008 1.00 92.58	N
		13.240 61.536 153.297 1.00 89.00	C
		14.176 62.663 153.687 1.00 86.59	
ATOM	3146 O LEUB 469	14.526 63.522 152.886 1.00 86.06	0
ATOM	3147 CB LEU B 469	11.775 61.857 153.578 1.00 89.46 14.614 62.658 154.934 1.00 84.75	С
ATOM	3151 N GLUB 470	14.614 62.658 154.934 1.00 84.75	N
ATOM	3152 CA GLUB 470	15.553 63.680 155.409 1.00 83.83	C
ATOM	3153 C GLUB 470	16.940 63.374 154.870 1.00 79,82	С
ATOM	3154 O GLUB 470	17.699 64.245 154.462 1.00 78.99	0
ATOM	3155 CB GLU B 470	15.408 63.750 156.913 1.00 88.01 16.703 63.787 157.705 1.00 93.53	С
ATOM	3156 CG GLUB 470	16.703 63.787 157.705 1.00 93.53	С
ATOM	3157 CD GLUB 470	16.434 63.541 159.185 1.00 97.16	С
		15.314 63.053 159.516 1.00 98.71	
ATOM	3159 OE2 GLU B 470	17.365 63.849 159.982 1.00 99.17	0
ATOM	3160 N GLUB 471	17.323 62.106 154.807 1.00 75.78 18.593 61.660 154.266 1.00 71.86	N
ATOM	3161 CA GLUB 471	18,593 61,660 154,266 1,00 71.86	С
ATOM	3162 C GLUB 471	18.605 62.021 152.775 1.00 70.49	C
		19.582 62.544 152.244 1.00 71.13	0
ATOM	3164 CB GLUB 471	18 795 60 156 154 404 1 00 70 33	С
ATOM	3165 CG GLUB 471	18 983 59 604 155 781 1 00 69 51	C
ATOM	3166 CD GLUB 471	18.983 59.604 155.781 1.00 69.51 20.401 59.447 156.253 1.00 69.90	Č
ATOM	3167 OF1 GLUB 471	21.123 58.551 155.784 1.00 69.90	Ō
		20.888 60.204 157.125 1.00 70.61	Ö
		17.512 61.755 152.064 1.00 68.23	N
		17.443 62.094 150.661 1.00 66.98	C
ATOM	3171 C LYS B 472	17.599 63.591 150.478 1.00 65.63	c
ATOM	3172 O I VS B 472	18.392 63.964 149.607 1.00 65.62	Ö
		16.170 61.590 150.011 1.00 68.62	C
		16.125 60.081 149.849 1.00 71.13	Č
	3175 CD LYS B 472	15.015 59.682 148.893 1.00 74.04	č
	3176 CE LYS B 472	14.408 58.333 149.248 1.00 76.38	č
	3177 NZ LYS B 472	15.152 57.157 148.664 1.00 77.87	N
	3178 N ASP B 473	16.920 64.440 151.237 1.00 64.78	N
	3179 CA ASP B 473	17.082 65.877 151.034 1.00 65.36	C
	3180 C ASP B 473	18.516 66.332 151.232 1.00 62.76	c
		19.109 67.035 150.430 1.00 63.80	0
	3181 O ASP B 473		
	3182 CB ASP B 473	16.291 66.752 152.000 1.00 69.33	C C
	3183 CG ASP B 473		
	3184 OD1 ASP B 473	14.441 65.701 150.904 1.00 76.03	0
	3185 OD2 ASP B 473	14.069 67.050 152.657 1.00 76.73	0
	3186 N HIS B 474	19.072 65.908 152.354 1.00 59.23	N
		20.449 66.243 152.659 1.00 56.40	C
AIUM	3188 C HIS B 474	21.328 65.998 151.428 1.00 55.19	С

WU	76/3001	4	181/371	
ATO) (2100	O LITE D A7A	22.045 66.881 150.947 1.00 53.51	0
		O HIS B 474	20.887 65.360 153.835 1.00 55.62	C
		CB HIS B 474	22,279 65.818 154.180 1.00 56.07	C
		CG HIS B 474		N
		ND1 HIS B 474	22.540 67.145 154.498 1.00 55.48	C
		CD2 HIS B 474	23.435 65.111 154.203 1.00 56.58	C
		CE1 HIS B 474	23.843 67.220 154.730 1.00 56.88	
		NE2 HIS B 474	24.410 66.017 154.559 1.00 57.47	N
		N ILEB 475	21.250 64.758 150.917 1.00 54.03	N
		CA ILE B 475	22.003 64.377 149.746 1.00 53.42	C
ATOM		C ILE B 475	21.668 65.281 148.572 1.00 53.75	C
ATOM		O ILE B 475	22.569 65.802 147.901 1.00 52.81	0
		CB ILE B 475	21.753 62.918 149.374 1.00 53.33	C
		CG1 ILE B 475	22.378 62.047 150.462 1.00 53.70	C
		CG2 ILE B 475	22.370 62.593 148.021 1.00 53.57	C
		CD1 ILE B 475	22.291 60.573 150.105 1.00 54.14	С
		N HISB 476	20.391 65.533 148.302 1.00 54.79	N
		CA HISB 476	20.092 66.414 147.169 1.00 57.16	С
		C HIS B 476	20.729 67.776 147.357 1.00 58.28	C
		O HIS B 476	21.293 68.396 146.440 1.00 58.61	O
		CB HIS B 476	18.596 66.470 146.957 1.00 59.37	С
ATOM	3209	CG HIS B 476	18.080 65.206 146.317 1.00 61.81	С
		ND1 HIS B 476	18.745 64.600 145.267 1.00 62.78	N
ATOM	3211	CD2 HIS B 476	16.989 64.450 146.584 1.00 61.95	С
ATOM	3212	CE1 HIS B 476	18.057 63.517 144.922 1.00 63.31	C
ATOM	3213	NE2 HIS B 476	16.995 63.403 145.701 1.00 62.29	N
ATOM	3214	N ARG B-477	20.681 68.281 148.587 1.00 59.16	N
ATOM	3215	CA ARG B 477	21.236 69.547 148.986 1.00 58.98	С
ATOM	3216	C ARG B 477	22.726 69.681 148.710 1.00 57.17	С
ATOM	3217	O ARG B 477	23.164 70.678 148.124 1.00 56.93	0
ATOM	3218	CB ARG B 477	21.033 69.701 150.492 1.00 62.77	С
ATOM	3219	CG ARG B 477	20.678 71.151 150.807 1.00 69.05	С
ATOM	3220	CD ARG B 477	19.157 71.257 150.564 1.00 74.67	С
		NE ARG B 477		N
ATOM	3222	CZ ARG B 477		С
ATOM	3223	NH1 ARG B 477		N
ATOM	3224	NH2 ARG B 477	17.848 69.972 153.749 1.00 83.97	N
ATOM	3225	N VAL B 478	23.494 68.680 149.141 1.00 54.36	N
ATOM	3226	CA VAL B 478	24.943 68.675 148.939 1.00 52.49	С
ATOM	3227	C VAL B 478	25.235 68.604 147.450 1.00 52.18	С
ATOM	3228	O VAL B 478	26.104 69.239 146.842 1.00 51.94	O.
ATOM	3229	CB VAL B 478	25.543 67.480 149.693 1.00 52.54	С
		CG1 VAL B 478	27.053 67.386 149.590 1.00 52.18	С
		CG2 VAL B 478	25.113 67.585 151.156 1.00 53.20	С
		N LEUB 479	24.407 67.803 146.763 1.00 51.49	N
		CA LEU B 479	24,513 67.646 145.311 1.00 49.86	С

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			180 (10)	
ATOM	3234	C LEU B 479	24.395 69.020 144.666 1.00 50.12	С
ATOM	3235	O LEU B 479	25.165 69.295 143.740 1.00 50.39	Ο
ATOM	3236	CB LEU B 479	23.496 66.630 144.787 1.00 46.59	С
ATOM	3237	CG LEU B 479	23.998 65.183 144.867 1.00 44.76	С
ATOM	3238	CD1 LEU B 479	22.873 64.231 144.537 1.00 44.80	С
ATOM	3239	CD2 LEU B 479	25.182 64.961 143.942 1.00 44.34	С
ATOM	3240	N ASP B 480	23.478 69.860 145.159 1.00 50.73	N
ATOM	3241	CA ASP B 480	23.365 71.196 144.568 1.00 52.25	С
ATOM	3242	C ASP B 480	24.633 71.994 144.842 1.00 52.37	С
ATOM	3243	O ASP B 480	25.177 72.652 143.956 1.00 51.99	0
ATOM	3244	CB ASP B 480	22.148 71.963 145.047 1.00 53.28	С
ATOM	3245	CG ASP B 480	20.835 71.318 144.638 1.00 54.67	С
ATOM	3246	OD1 ASP B 480	20.799 70.546 143.657 1.00 55.26	0
ATOM	3247	OD2 ASP B 480	19.791 71.559 145.291 1.00 55.41	О
ATOM	3248	N LYS B 481	25.139 71.893 146.064 1.00 53.75	N
ATOM	3249	CA LYS B 481	26.357 72.608 146.440 1.00 54.79	С
ATOM	3250	C LYS B 481	27.474 72.167 145.520 1.00 54.09	C
ATOM	3251	O LYS B 481	28.165 73.015 144.955 1.00 55.38	0
ATOM	3252	CB LYS B 481	26.743 72.364 147.889 1.00 58.10	С
ATOM	3253	CG LYS B 481	27.789 73.346 148.394 1.00 62.90	С
ATOM	3254	CD LYS B 481	27.145 74.541 149.106 1.00 66.84	С
ATOM		CE LYS B 481	27.999 75.805 149.020 1.00 69.39	С
ATOM		NZ LYS B 481	29.024 75.782 147.919 1.00 71.15	N
ATOM	3257	N ILE B 482	27.646 70.855 145.320 1.00 52.58	N
ATOM		CA ILE B 482	28.705 70.401 144.407 1.00 50.25	С
ATOM	3259	C ILE B 482	28.406 70.935 143.020 1.00 49.16	С
ATOM		O ILE B 482	29.350 71.353 142.339 1.00 49.20	Ο
ATOM	3261	CB ILE B 482	28.917 68.898 144.435 1.00 49.88	С
ATOM		CG1 ILE B 482	29.455 68.527 145.825 1.00 50.32	С
ATOM			29.934 68.446 143.417 1.00 49.96	С
ATOM			28.834 67.247 146.349 1.00 51.02	С
ATOM		N THR B 483		N
			26.874 71.594 141.288 1.00 49.74	С
		C THR B 483	27.393 73.030 141.196 1.00 51.14	С
		O THR B 483	28.129 73.405 140.265 1.00 51.11	Ο
		CB THR B 483	25.368 71.577 141.003 1.00 48.94	С
ATOM		OG1 THR B 483	25.050 70.188 140.912 1.00 49.10	О
ATOM		CG2 THR B 483	25.071 72.316 139.717 1.00 49.01	С
ATOM		N ASP B 484	27.017 73.834 142.213 1.00 51.19	N
ATOM		CA ASP B 484	27.476 75.218 142.294 1.00 50.56	С
ATOM		C ASP B 484	29.002 75.268 142.245 1.00 50.46	С
ATOM		O ASP B 484	29.605 76.073 141.522 1.00 51.67	О
ATOM		CB ASP B 484	27.001 75.898 143.558 1.00 50.97	C
ATOM		CG ASP B 484	25.487 76.070 143.586 1.00 53.30	С
ATOM	3278	OD1 ASP B 484	24.853 75.982 142.497 1.00 53.11	0

183/371 24.940 76.307 144.717 1.00 53.76 ATOM 3279 OD2 ASP B 484 0 ATOM 3280 N THR B 485 29.694 74.386 142.956 1.00 49.24 N 31.154 74.396 142.907 1.00 49.60 C ATOM 3281 CA THR B 485 C ATOM 3282 C THR B 485 31.680 74.196 141.495 1.00 50.42 ATOM 3283 O THR B 485 32.684 74.791 141.087 1.00 50.51 O 31.664 73.271 143.835 1.00 48.97 C ATOM 3284 CB THR B 485 ATOM 3285 OG1 THR B 485 30.967 73.451 145.080 1.00 47.88 0 33.176 73.286 143.960 1.00 47.44 Ċ ATOM 3286 CG2 THR B 485 ATOM 3287 N LEUB 486 31,002 73,328 140,741 1.00 51.30 N 31.433 73.036 139.368 1.00 51.82 C ATOM 3288 CA LEUB 486 ATOM 3289 C LEU B 486 31.339 74.277 138.479 1.00 52.24 C 32,257 74,683 137,774 1.00 50.69 0 ATOM 3290 O LEUB 486 ATOM 3291 CB LEU B 486 30.573 71.907 138.761 1.00 49.64 C 31.218 70.532 138.888 1.00 48.31 ATOM 3292 CG LEUB 486 ATOM 3293 CD1 LEU B 486 30.237 69.504 138.358 1.00 48.07 C 32,555 70.536 138.164 1.00 47.39 C ATOM 3294 CD2 LEU B 486 N ATOM 3295 N ILE B 487 30.147 74.897 138.557 1.00 53.50 ATOM 3296 CA ILE B 487 29.921 76.092 137.754 1.00 55.16 C ATOM 3297 C ILE B 487 30.953 77.157 138.134 1.00 57.21 C ATOM 3298 O ILE B 487 31.609 77.809 137.322 1.00 57.31 0 ATOM 3299 CB ILE B 487 28.510 76.631 137.978 1.00 54.14 \mathbf{C} 27.457 75.695 137.432 1.00 54.26 C ATOM 3300 CG1 ILE B 487 C ATOM 3301 CG2 ILE B 487 28.458 77.994 137.316 1.00 55.14 C 27.219 75.771 135.943 1.00 54.81 ATOM 3302 CD1 ILE B 487 31.105 77.327 139.446 1.00 58.96 N ATOM 3303 N HIS B 488 ATOM 3304 CA HIS B 488 32.052 78.277 139.982 1.00 60.55 C ATOM 3305 C HIS B 488 33.385 78.041 139.302 1.00 60.12 ATOM 3306 O HIS B 488 33,987 78,945 138,743 1.00 61.16 O ATOM 3307 CB HIS B 488 32.201 78.053 141.481 1.00 63.98 C ATOM 3308 CG HIS B 488 33.356 78.861 142.005 1.00 67.76 ATOM 3309 ND1 HIS B 488 33.313 80.239 142.060 1.00 68.99 N C 34.573 78.457 142.475 1.00 69.21 ATOM 3310 CD2 HIS B 488 ATOM 3311 CE1 HIS B 488 34.481 80.641 142.565 1.00 70.75 Ċ 35.266 79.590 142.831 1.00 70.44 N ATOM 3312 NE2 HIS B 488 33,870 76,808 139,343 1.00 59.86 N ATOM 3313 N LEUB 489 35.140 76.503 138.700 1.00 60.03 C ATOM 3314 CA LEU B 489 35.214 76.966 137.242 1.00 60.16 ATOM 3315 C LEUB 489 C 36.162 77.570 136.755 1.00 58.98 ATOM 3316 O LEUB 489 0 C ATOM 3317 CB LEUB 489 35.311 74.975 138.755 1.00 58.86 35.797 74.471 140.096 1.00 59.40 C ATOM 3318 CG LEUB 489 35.741 72.942 140.083 1.00 60.90 ATOM 3319 CD1 LEU B 489 C C ATOM 3320 CD2 LEU B 489 37.209 74.937 140.395 1.00 59.49 ATOM 3321 N MET B 490 34.193 76.643 136.465 1.00 61.21 N 34.106 76.937 135.052 1.00 62.35 C ATOM 3322 CA MET B 490 ATOM 3323 C MET B 490 34.095 78.425 134.725 1.00 62.90 C

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			(D-/ 10	
ATOM		O MET B 490		О
ATOM			32.807 76.321 134 - O0 1.00 62.53	С
ATOM	3326	CG MET B 490	33.018 74.922 133 939 1.00 62.79	С
ATOM		SD MET B 490	31.400 74.130 133.827 1.00 64.70	S
ATOM		CE MET B 490	31.840 72.442 134.233 1.00 63.89	С
ATOM		N ALA B 491	33.336 79.163 135.541 1.00 63.19	N
ATOM	3330	CA ALA B 491	33.245 80.608 135.353 1.00 63.40	С
ATOM	3331	C ALA B 491	34.665 81.115 135.583 1.00 63.75	С
ATOM	3332	O ALA B 491	35.219 81.807 134.739 1.00 63.44	Ο
ATOM	3333	CB ALA B 491	32.252 81.242 136.296 1.00 63.10	С
ATOM	3334	N LYS B 492	35.288 80.683 136.678 1.00 64.63	N
ATOM	3335	CA LYS B 492	36.662 81.082 136.954 1.00 66.16	С
ATOM	3336	C LYS B 492	37.545 80.773 135.765 1.00 66.57	С
ATOM	3337	O LYS B 492	38.458 81.559 135.514 1.00 68.67	О
		CB LYSB 492	37.235 80.489 138.236 1.00 66.65	С
ATOM	3343	N ALA B 493	37.346 79.758 134.952 1.00 67.06	N
		CA ALA B 493	38.181 79.515 133.784 1.00 68.05	С
		C ALA B 493	37.649 80.371 132.632 1.00 69.31	С
		O ALA B 493	38.043 80.265 131.472 1.00 70.45	О
ATOM		CB ALA B 493	38.217 78.061 133.355 1.00 67.81	С
ATOM		N GLY B 494	36.705 81.254 132.897 1.00 69.82	N
		CA GLY B 494		С
		C GLY B 494	35.391 81.444 130.819 1.00 70.48	C
		O GLY B 494	35.767 81.599 129.655 1.00 72.21	0
		N LEUB 495	34.359 80.656 131.074 1.00 70.34	N
ATOM		CA LEUB 495	33.646 80.047 129.944 1.00 69.20	С
ATOM		C LEU B 495	32.365 80.888 129.907 1.00 68.78	C
ATOM		O LEUB 495		0
		CB LEUB 495		C
		CG LEU B 495		C
		CD1 LEU B 495	33.750 76.182 130.417 1.00 69.36	C
ATOM			35.598 77.732 129.809 1.00 69.12	C
ATOM		N THR B 496		N
			30.574 81.867 128.685 1.00 70.03	C
		C THR B 496	29,554 81.192 129.572 1.00 70.46	C
ATOM			29.688 80.016 129.897 1.00 71.40	0
		CB THR B 496	29.987 81.709 127.275 1.00 70.86	C
		OG1 THR B 496	30.999 82.069 126.332 1.00 72.15	0
		CG2 THR B 496	28.731 82.529 127.084 1.00 72.22	C
		N LEUB 497	28.476 81.872 129.917 1.00 71.30	N
		CA LEU B 497	27.413 81.282 130.717 1.00 71.94	C
		C LEUB 497	26.818 80.089 129.961 1.00 72.66	C
		O LEUB 497	26.362 79.078 130.509 1.00 72.74	0
		CB LEU B 497	26.361 82.336 130.938 1.00 73.14	C
ATOM	3372	CG LEUB 497	25.737 82.520 132.308 1.00 75.05	С

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			185/371	
ATOM	3373	CD1 LEU B 497	24.213 82.497 132.169 1.00 75.56	С
ATOM		CD2 LEU B 497	26.223 81.553 133.368 1.00 75.08	С
ATOM		N GLN B 498	26.801 80.172 128.628 1.00 73.15	N
		CA GLN B 498	26.286 79.097 127.802 1.00 73.20	С
		C GLN B 498	27.304 77.965 127.748 1.00 71.99	C
ATOM	3378	O GLN B 498	26.873 76.805 127.766 1.00 73.27	Ο
ATOM	3379	CB GLN B 498	25,909 79,531 126,397 1.00 75.34	С
ATOM	3380	CG GLN B 498	25.953 78.364 125.417 1.00 78.94	С
ATOM	3381	CD GLN B 498	25.355 78.648 124.062 1.00 81.48	С
ATOM	3382	OE1 GLN B 498	24.595 77.837 123.510 1.00 82.87	Ο
ATOM	3383	NE2 GLN B 498	25.686 79.809 123.489 1.00 82.87	N
	3384	N GLN B 499	28.602 78.215 127.695 1.00 69.54	N
		CA GLN B 499	29.551 77.094 127.692 1.00 67.99	С
ATOM	3386	C GLN B 499	29.514 76.401 129.062 1.00 66.82	С
ATOM	3387	O GLN B 499	29.697 75.198 129.245 1.00 66.87	О
		CB GLN B 499	30.965 77.605 127.473 1.00 68.69	С
		CG GLN B 499	30.951 78.798 126.524 1.00 70.30	C
		CD GLN B 499	32.354 79.028 126.007 1.00 71.96	C
		OE1 GLN B 499	33.200 79.505 126.773 1.00 73.64	0
		NE2 GLN B 499	32.534 78.653 124.749 1.00 72.63	N
		N GLNB 500	29.260 77.202 130.100 1.00 64.43	N
		CA GLN B 500	29.153 76.673 131.436 1.00 62.40	С
		C GLN B 500	28.025 75.641 131.437 1.00 60.46	C
		O GLN B 500	28.339 74.482 131.749 1.00 60.49	0
ATOM		CB GLN B 500	28.855 77.755 132.459 1.00 62.93	C C
ATOM		CG GLN B 500	30.091 78.493 132.957 1.00 63.99	C
		CD GLN B 500	29.637 79.803 133.582 1.00 65.12	_
		OE1 GLN B 500	28.785 79.839 134.472 1.00 65.59	0 N
		NE2 GLN B 500	30.208 80.896 133.098 1.00 65.97	N N
ATOM		N HIS B 501	26.791 76.028 131.071 1.00 57.49	·C
ATOM		CA HIS B 501	25.743 74.994 131.086 1.00 55.77 25.983 73.824 130.128 1.00 55.13	C
		C HIS B 501	25.543 72.698 130.416 1.00 55.20	0
		O HIS B 501 CB HIS B 501	24.363 75.550 130.938 1.00 55.37	C
		CG AHIS B 501	23.935 76.140 129.646 0.50 55.16	C
		CG BHIS B 501	24.021 76.821 131.635 0.50 55.88	č
		ND1AHIS B 501	23.174 77.302 129.600 0.50 55.27	N
		ND1BHIS B 501	24.177 76.981 132.992 0.50 56.03	N
		CD2AHIS B 501	24.110 75.752 128.363 0.50 54.82	C
		CD2BHIS B 501	23.524 77.993 131.170 0.50 55.80	Č
		CE1AHIS B 501	22.917 77.598 128.336 0.50 54.98	Č
		CEIBHIS B 501	23.800 78.200 133.332 0.50 56.19	Č
		NE2AHIS B 501	23.477 76.674 127.566 0.50 54.81	N
		NE2BHIS B 501	23.403 78.836 132.241 0.50 56.01	N
		N GLN B 502	26.669 73.995 129.009 1.00 53.45	N
	J-717	02112		

wo	98/5681	2	,	PCT/GI
			186/371	
ATOM	3418	CA GLN B 502	26.940 72.871 128.127 1.00 52.90	С
ATOM		C GLN B 502	27.942 71.918 128.772 1.00 52.22	С
ATOM	3420	O GLN B 502	27.647 70.721 128.922 1.00 51.61	О
		CB GLN B 502	27.422 73.419 126.787 1.00 54.22	C
		CG GLN B 502	26.373 74.342 126.184 1.00 55.11	C
		CD GLN B 502	26.499 74.615 124.704 1.00 54.93	C
		OE1 GLN B 502	27.619 74.599 124.169 1.00 55.67	0
		NE2 GLN B 502	25.343 74.862 124.089 1.00 53.79	N N
		N ARG B 503	29.108 72.384 129.218 1.00 50.84 30.092 71.560 129.898 1.00 48.49	C
		CA ARG B 503 C ARG B 503	29.463 70.800 131.069 1.00 48.40	C
ATOM		O ARG B 503	29.729 69.604 131.216 1.00 49.87	Ö
ATOM		CB ARG B 503	31.217 72.421 130.495 1.00 47.02	Č
		CG ARG B 503	32.435 71.558 130.785 1.00 47.10	Č
		CD ARG B 503	33.700 72.366 130.968 1.00 45.82	č
		NE ARG B 503	34.788 71.588 131.542 1.00 45.26	N
		CZ ARG B 503	35.665 70.918 130.815 1.00 46.26	С
		NH1 ARG B 503	35.568 70.910 129.493 1.00 46.31	N
ATOM	3436	NH2 ARG B 503	36.669 70.235 131.366 1.00 47.52	N
		N LEUB 504	28.644 71.462 131.888 1.00 46.45	N
		CA LEU B 504	28.023 70.802 133.014 1.00 45.17	С
		C LEUB 504	27.339 69.548 132.495 1.00 46.22	C
ATOM		O LEUB 504	27.695 68.426 132.869 1.00 47.23	0
ATOM		CB LEU B 504	27.017 71.705 133.720 1.00 43.90	C
		CG LEU B 504	26.422 71.152 135.018 1.00 43.02	C C
ATOM		CD1 LEU B 504	27.484 70.796 136.035 1.00 42.09 25.434 72.161 135.603 1.00 42.49	C
		CD2 LEU B 504 N ALA B 505	26.384 69.771 131.586 1.00 46.57	N
		CA ALA B 505	25.639 68.658 130.986 1.00 45.30	Ċ
		C ALA B 505	26,622 67,677 130.371 1.00 46.91	Č
		O ALA B 505	26.518 66.469 130.660 1.00 48.20	O
		CB ALAB 505	24.658 69.248 130.021 1.00 44.08	С
		N GLN B 506	27.629 68.077 129.585 1.00 47.50	N
ATOM	3451	CA GLN B 506	28.566 67.094 129.051 1.00 47.74	С
ATOM	3452	C GLN B 506	29.206 66.326 130.190 1.00 48.34	С
		O GLN B 506	29.273 65.098 130.031 1.00 50.56	0
		CB GLN B 506	29.642 67.637 128.122 1.00 48.83	C
		CG AGLN B 506	29.324 68.944 127.440 0.50 49.79	C
		CG BGLN B 506	29.073 68.052 126.764 0.50 49.57	C
		CD AGLN B 506	30.244 69.417 126.351 0.50 50.30	C C
		CD BGLN B 506	28.599 66.920 125.870 0.50 49.56 31.471 69.382 126.470 0.50 50.66	0
		OE1AGLN B 506 OE1BGLN B 506	29.020 65.770 126.068 0.50 50.14	0
		NE2AGLN B 506	29.672 69.881 125.241 0.50 50.69	N
		NE2BGLN B 506	27.744 67.233 124.896 0.50 48.23	N
VION	J-102		27,777 07,200 121,070 0.00 10,20	- '

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ATOM	3463	N LEUB 507	29.637 66.940 131.278 1.00 48.08	N
		CA LEU B 507	30.249 66.175 132.359 1.00 48.18	С
ATOM	3465	C LEU B 507	29.274 65.201 132.999 1.00 47.50	С
ATOM	3466	O LEUB 507	29.611 64.010 133.075 1.00 49.50	0
ATOM	3467	CB LEU B 507	30.821 67.077 133.452 1.00 49.39	С
ATOM	3468	CG LEU B 507	32.048 67.900 133.026 1.00 50.17	С
ATOM	3469	CD1 LEU B 507	32.468 68.844 134.135 1.00 49.83	С
ATOM	3470	CD2 LEU B 507	33.163 66.965 132.590 1.00 50.59	С
ATOM	3471	N LEUB 508	28.108 65.661 133.416 1.00 45.18	N
ATOM	3472	CA LEUB 508	27.146 64.743 134.024 1.00 44.33	С
ATOM	3473	C LEU B 508	26.695 63.653 133.076 1.00 44.72	С
ATOM	3474	O LEU B 508	26.456 62.520 133.573 1.00 46.18	Ο
ATOM	3475	CB LEU B 508	25.969 65.562 134.561 1.00 43.86	С
ATOM	3476	CG LEU B 508	26.418 66.604 135.595 1.00 44.31	С
ATOM	3477	CD1 LEU B 508	25.304 67.481 136.094 1.00 44.65	С
ATOM	3478	CD2 LEU B 508	27.001 65.893 136.814 1.00 46.31	С
ATOM	3479	N LEUB 509	26.631 63.860 131.740 1.00 42.70	N
		CA LEU B 509	26.188 62.738 130.907 1.00 41.76	С
		C LEU B 509		С
		O LEU B 509		О
			25.771 63.111 129.500 1.00 39.78	С
		CG LEU B 509	24.498 63.933 129.331 1.00 39.38	С
		CD1 LEU B 509	24.376 64.378 127.887 1.00 39.53	C
		CD2 LEU B 509	23.261 63.183 129.768 1.00 38.89	С
		N ILE B 510	28.452 61.794 131.175 1.00 42.74	N
		CA ILEB 510	29.430 60.702 131.201 1.00 42.35	С
		C ILE B 510	29.081 59.803 132.385 1.00 41.76	C
		O ILE B 510	29.280 58.577 132.334 1.00 41.62	0
ATOM	-		30.874 61.227 131.277 1.00 42.40	C
			31.414 61.613 129.902 1.00 43.54	C
			31.861 60.190 131.777 1.00 42.50	C
		_	32.106 62.960 129.894 1.00 45.42	C
ATOM		N LEUB 511	28.525 60.389 133.451 1.00 40.66	N
		CA LEUB 511	28.170 59.585 134.616 1.00 42.25	C
		C LEUB 511	27.297 58.398 134.249 1.00 42.82	C
		O LEUB 511	27.463 57.267 134.735 1.00 43.36	0
		CB LEUB 511	27.601 60.448 135.730 1.00 42.09	C
		CG LEUB 511	28.535 61.542 136.285 1.00 41.35	C
		CD1 LEU B 511	27.865 62.131 137.519 1.00 41.68	C
		CD2 LEU B 511	29.923 61.032 136.646 1.00 39.19	C
		N SER B 512	26.357 58.553 133.328 1.00 42.90	N
		CA SER B 512	25.559 57.466 132.826 1.00 42.26	C
		C SER B 512	26.408 56.302 132.306 1.00 42.66	C
		O SER B 512	26.211 55.124 132.655 1.00 43.46	0
ATOM	3507	CB SER B 512	24.841 57.983 131.565 1.00 43.15	С

25.173 50.053 130.179 1.00 40.24

27.202 50.108 129.400 1.00 41.00

25.303 49.066 129.336 1.00 39.65

26.514 49.070 128.834 1.00 39.98

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ATOM 3549 ND1 HIS B 516

ATOM 3550 CD2 HIS B 516

ATOM 3551 CE1 HIS B 516

ATOM 3552 NE2 HIS B 516

WC	98/56812		PCT
		189/371	
ATOM	3553 N MET B 5		N
	3554 CA MET B		С
ATOM	3555 C MET B 5	17 30.489 49.440 133.998 1.00 42.00	С
	3556 O MET B 5		0
	3557 CB MET B :		C
	3558 CG MET B		C
	3559 SD MET B :		S
	3560 CE MET B :		C
ATOM	3561 N SER B 51		N
ATOM	3562 CA SER B 5		C C
ATOM	3563 C SER B 51		0
ATOM ATOM	3564 O SER B 51 3565 CB SER B 5		C
	3566 OG SER B 5		Ö
ATOM			N
	3568 CA ASN B 5		C
	3569 C ASN B 5		C
	3570 O ASN B 5		Ο
	3571 CB ASN B 5		С
	3572 CG ASN B 5		C
	3573 OD1 ASN B		0
ATOM	3574 ND2 ASN B		N
ATOM	3575 N LYS B 52		N
ATOM			C C
	3577 C LYS B 52 3578 O LYS B 52		o
ATOM ATOM	3579 CB LYS B 5		Č
	3580 CG LYS B 5		Č
	3581 CD LYS B 5		Č
	3582 CE LYS B 5		С
	3583 NZ LYS B 5		N
ATOM	3584 N GLY B 5	21 30.957 45.705 134.659 1.00 44.61	N
	3585 CA GLY B		С
	3586 C GLY B 5		C
	3587 O GLY B 5		0
	3588 N MET B 5		N
	3589 CA MET B		C C
	3590 C MET B 5 3591 O MET B 5		0
	3591 O MET B 3		C
	3593 CG MET B		Č
	3594 SD METB		S
	3595 CE MET B		Ċ
	3596 N GLUB 5		N
	3597 CA GLUB:		С

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		190/371	
ATOM	3598 C GLUB 523	29.801 40.335 135.793 1.00 48.34	С
ATOM	3599 O GLUB 523	29.842 39.152 136.111 1.00 48.80	0
ATOM	3600 CB GLU B 523	27.693 41.477 134.926 1.00 56.32	С
ATOM	3601 CG GLU B 523	26.222 41.586 135.253 1.00 63.90	C
	3602 CD GLU B 523		С
ATOM	3603 OE1 GLU B 523	26.274 39.292 136.084 1.00 72.07	О
ATOM	3604 OE2 GLU B 523	24.573 40.579 136.664 1.00 72.34	0
	3605 N HIS B 524		N
ATOM	3606 CA HIS B 524	32.042 40.187 134.925 1.00 44.63	С
ATOM	3607 C HIS B 524	32.786 39.694 136.136 1.00 45.63	С
ATOM	3608 O HIS B 524	33.174 38.530 136.210 1.00 46.13	0
ATOM	3609 CB HIS B 524	32.941 41.153 134.131 1.00 44.39	С
ATOM	3610 CG HISB 524	34.264 40.554 133.809 1.00 45.05	С
ATOM	3611 ND1 HIS B 524	35.340 40.624 134.677 1.00 46.06	N
ATOM	3612 CD2 HIS B 524	34.689 39.871 132.727 1.00 45.55	C
		36.379 40.011 134.130 1.00 46.99	С
ATOM	3614 NE2 HIS B 524	36.014 39.538 132.934 1.00 46.65	N
	3615 N LEUB 525		N
		33.838 40.173 138.305 1.00 48.66	С
ATOM	3617 C LEUB 525	33.186 38.970 138.973 1.00 51.45	С
		33.801 38.061 139.503 1.00 51.39	0
ATOM	3619 CB LEU B 525	34.009 41.328 139.283 1.00 47.23	С
		34.669 40.941 140.610 1.00 46.40	С
		36.099 40.533 140.321 1.00 46.02	C ·
	3622 CD2 LEU B 525		С
	3623 N TYR B 526	31.860 39.006 138.936 1.00 54.54	N
	3624 CA TYR B 526	31.029 37.963 139.465 1.00 58.05	C
	3625 C TYR B 526		C
ATOM			0
		29.591 38.447 139.352 1.00 60.78	C
	3628 CG TYR B 526	28.713 37.388 139.962 1.00 64.37	C
	3629 CD1 TYR B 526		C
	3630 CD2 TYR B 526		C
	3631 CE1 TYR B 526	27.700 36.427 141.916 1.00 68.78	C
	3632 CE2 TYR B 526	27.300 35.457 139.738 1.00 69.50	C
	3633 CZ TYR B 526	27.112 35.477 141.106 1.00 70.89	C
	3634 OH TYR B 526	26.313 34.509 141.697 1.00 74.25	0
	3635 N SER B 527	31.261 36.673 137.336 1.00 60.47	N
	3636 CA SER B 527	31.498 35.385 136.667 1.00 61.49	C
	3637 C SER B 527	32.948 35.014 136.945 1.00 61.49	C
	3638 O SER B 527	33.157 33.877 137.371 1.00 62.15	0
	3639 CB SER B 527	31.192 35.377 135.188 1.00 62.44	С
	3640 OG SER B 527	31.689 36.588 134.634 1.00 63.98	O
	3641 N MET B 528	33.911 35.911 136.843 1.00 61.64	N
ATOM	3642 CA MET B 528	35.281 35.555 137.196 1.00 63.8°	С

wo	98/568 1	12	191/371	PCT/GB98/01708
A TO 3.4	2642	C MET B 528	35.329 34.828 138.542 1.00 64.80	С
		O MET B 528	36.067 33.868 138.753 1.00 63.49	
			36.167 36.800 137.243 1.00 64.77	
			36.878 37.227 135.984 1.00 65.29	
ATOM	3647	SD MET B 528	37.201 35.912 134.760 1.00 66.35	S
		CE MET B 528	35.670 36.008 133.820 1.00 65.10	C
		N LYS B 529	34.553 35.264 139.522 1.00 67.52	N
		CA LYS B 529	34.492 34.654 140.833 1.00 70.80	C
		C LYS B 529	33.860 33.273 140.754 1.00 72.85	C
		O LYS B 529	34.298 32.357 141.450 1.00 73.96	Ō
			33.705 35.538 141.795 1.00 71.14	C
			32.734 34.819 142.692 1.00 72.73	С
ATOM	3655	CD LYS B 529	32.855 35.292 144.119 1.00 75.27	
ATOM	3656	CE LYS B 529	31.706 34.773 144.975 1.00 77.62	С
ATOM	3657	NZ LYSB 529	30.380 34.816 144.286 1.00 78.57	N
		N CYS B 530		N
			32.150 31.817 139.833 1.00 78.47	С
		C CYS B 530	33.059 30.823 139.165 1.00 80.04	С
ATOM	3661	O CYS B 530	33.123 29.653 139.549 1.00 81.22	0
ATOM	3662	CB CYS B 530	30.800 32.058 139.165 1.00 79.44	С
ATOM	3663	SG ACYS B 530	29.756 32.972 140.357 0.50 80.86	S
ATOM	3664	SG BCYS B 530	29.435 31.171 139.942 0.50 81.98	S
			33.878 31.218 138.207 1.00 81.81	N
			34.846 30.378 137.528 1.00 83.72	С
ATOM	3667	C LYS B 531	36.034 30.069 138.439 1.00 85.03	C ,
ATOM			37.009 29.407 138.089 1.00 85.56	0
			35.405 31.112 136.302 1.00 84.17	С
			34.640 30.945 135.014 1.00 85.13	
			33.167 31.305 135.153 1.00 86.04	
			36.050 30.578 139.651 1.00 86.77	N
			37.099 30.391 140.629 1.00 88.41	С
		C ASN B 532	38.429 30.832 140.066 1.00 87.48	C
		O ASN B 532	39.358 30.052 139.939 1.00 88.95	0
		CB ASN B 532	37.128 28.922 141.046 1.00 91.42	C
		CG ASN B 532	35.880 28.573 141.848 1.00 94.45	С
		OD1 ASN B 532	35.454 29.327 142.741 1.00 95.85	0
		ND2 ASN B 532	35.297 27.420 141.516 1.00 95.63	N
		N VAL B 533	38.555 32.084 139.686 1.00 86.02	N
		CA VAL B 533	39.753 32.676 139.116 1.00 84.42	C
		C VAL B 533	40.242 33.838 139.982 1.00 84.06	C
		O VAL B 533	41.369 34.303 140.067 1.00 84.64 39.383 33.246 137.730 1.00 83.89	O C
		CB VAL B 533 CG1 VAL B 533	40.659 33.683 137.031 1.00 83.89	C
ATOM		CG2 VAL B 533	38.598 32.275 136.875 1.00 83.22	C
		N VAL B 534	39.311 34.417 140.708 1.00 83.35	N
ATOM	3009	14 A UT 19 334	J9.511 J4.711 140.700 1.00 05.55	14

			193/3+1	
ATOM	3739	N LEU B 540	36.688 ⁴ 43.219 148.933 1.00 53.90	N
ATOM	3740	CA LEUB 540	36.181 43.177 147.572 1.00 52.79	С
ATOM	3741	C LEU B 540	34.995 42.215 147.482 1.00 53.01	С
ATOM	3742	O LEU B 540	33.997 42.532 146.834 1.00 51.76	Ο
ATOM	3743	CB LEU B 540	37.305 42.784 146.604 1.00 52.02	С
		CG LEUB 540		С
ATOM	3745	CD1 LEU B 540	36.882 44.150 144.556 1.00 50.14	С
		CD2 LEU B 540	37.918 41.898 144.288 1.00 49.04	С
		N LEU B 541	35.009 41.061 148.168 1.00 54.06	N
		CA LEU B 541	33.851 40.167 148.078 1.00 55.51	С
ATOM	3749	C LEU B 541	32.655 40.800 148.757 1.00 54.97	С
ATOM	3750	O LEU B 541	31.489 40.624 148.359 1.00 55.00	0
ATOM	3751	CB LEU B 541	34.142 38.728 148.519 1.00 57.67	С
ATOM	3752	CG LEU B 541	35.260 38.143 147.614 1.00 61.07	С
ATOM	3753	CD1 LEU B 541	35.784 36.793 148.069 1.00 62.23	С
ATOM	3754	CD2 LEU B 541	34.853 38.060 146.141 1.00 61.20	С
ATOM	3755	N GLU B 542	32.959 41.581 149.781 1.00 54.14	N
ATOM	3756	CA GLUB 542	31.900 42.280 150.518 1.00 53.44	С
ATOM	3757	C GLU B 542	31.240 43'.265 149.573 1.00 52.31	С
ATOM	3758	O GLU B 542	30.027 43.175 149.439 1.00 53.50	Ο
		CB GLUB 542	32.503 42.961 151.720 1.00 54.11	С
		CG GLUB 542	31.596 43.714 152.660 1.00 55.33	С
		CD GLUB 542	32.440 44.275 153.805 1.00 56.53	С
		OE1 GLU B 542	33.437 43.602 154.207 1.00 56.98	0
		OE2 GLU B 542	32.128 45.369 154.319 1.00 56.39	О
		N MET B 543	31.971 44.138 148.901 1.00 50.59	N
		CA MET B 543	31.349 45.101 148.005 1.00 49.97	С
ATOM		C MET B 543	30.635 44.411 146.876 1.00 50.80	C
ATOM	3767		29.540 44.816 146.450 1.00 52.14	0
ATOM		CB MET B 543		C
		CG MET B 543		C
		SD MET B 543		S
ATOM		CE MET B 543	31.905 47.356 151.033 1.00 52.76	С
		N LEU B 544	31.229 43.343 146.348 1.00 51.11	N
		CA LEUB 544	30.559 42.599 145.275 1.00 51.10	C
		C LEU B 544	29.248 42.015 145.783 1.00 52.28	C
		O LEU B 544	28.286 42.170 145.059 1.00 50.33	0
		CB LEUB 544	31.466 41.517 144.722 1.00 50.23	C
		CG LEU B 544	30.929 40.494 143.735 1.00 49.60	C
		CD1 LEU B 544	30.393 41.090 142.446 1.00 48.96	C
		CD2 LEU B 544	32.032 39.505 143.390 1.00 49.82	C
		N ASP B 545	29.195 41.388 146.960 1.00 56.16	N
		CA ASP B 545	27.967 40.810 147.477 1.00 60.23	C
		C ASP B 545	26.867 41.826 147.692 1.00 60.49	C
ATOM	3783	O ASP B 545	25.711 41.499 147.422 1.00 61.09	0
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ATOM 3784 CB ASP B		
ATOM 3785 CG ASP B	545 28.988 38.800 148.640 1.00 70 .11	l C
ATOM 3786 OD1 ASP E	3 545	
ATOM 3787 OD2 ASP B		
ATOM 3788 N ALAB		
ATOM 3789 CA ALA B		
ATOM 3790 C ALAB		
ATOM 3791 O ALAB		
ATOM 3792 CB ALA B		
ATOM 3793 N HIS B 5		
ATOM 3794 CA HISB		
ATOM 3795 C HISB 5		
ATOM 3796 O HIS B 5		
ATOM 3797 CB HIS B ATOM 3798 CG HIS B		
ATOM 3798 CO HIS B		
ATOM 3799 ND1 HIS B		
ATOM 3800 CE2 HIS B		
ATOM 3802 NE2 HIS B		
ATOM 3803 N ARGB		
ATOM 3804 CA ARGE		
ATOM 3805 C ARGB		
ATOM 3806 O ARGB		
ATOM 3807 CB ARG B		
ATOM 3808 CG ARGE		4 C
ATOM 3809 CD ARGE	548 26.909 40.087 142.494 1.00 92.8	5 C
ATOM 3810 NE ARGE	548 25.930 39.932 141.430 1.00 95.5	
ATOM 3811 CZ ARG B		
ATOM 3812 NH1 ARG	3 548 26.679 41.608 140.013 1.00 97.0	N 80
ATOM 3813 NH2 ARG	3 548 24.853 40.355 139.434 1.00 97.2	27 N
TER 3814 ARG B 54		
	3 600 40.756 47.434 139.452 1.00 35.7	
HETATM 3816 C2 EST I		
HETATM 3817 C3 EST I		
HETATM 3818 O3 EST		
HETATM 3819 C4 EST 1		
HETATM 3820 C5 EST 1		
HETATM 3821 C6 EST I		
HETATM 3822 C7 EST I		
HETATM 3823 C8 EST I		
HETATM 3824 C9 EST I		
HETATM 3825 C10 EST HETATM 3826 C11 EST		
HETATM 3827 C12 EST		
HETATM 3828 C13 EST		= -
ILLIAIWI 3020 CIJ ESI	D 000 37,330 44,210 137,337 1,00 34.	<i>33</i>

wo	98/56812	195/371	PCT/GB98
T TICTO A TO	M 3829 C14 EST B 600	37.537 45.388 136.370 1.00 34.22	С
		36.199 45.341 135.639 1.00 34.44	Č
		36.130 43.825 135.232 1.00 35.27	Č
	M 3832 C17 EST B 600	36.914 43.139 136.369 1.00 35.52	
		36.251 41.975 136.810 1.00 36.44	Ō
		36.270 44.480 138.386 1.00 33.93	C
	3835 N SER C 305	4.168 35.830 109.907 1.00 90.23	N
ATOM	3836 CA SER C 305	4.469 36.963 108.991 1.00 89.00	С
	3837 C SER C 305	3.303 37.261 108.070 1.00 88.50	С
ATOM	3838 O SER C 305	2.833 36.386 107.350 1.00 88.52	Ο
ATOM	3839 CB SER C 305	5.742 36.644 108.192 1.00 88.54	С
ATOM	3840 OG SER C 305	6.028 37.662 107.253 1.00 87.89	Ο
ATOM	3841 N LEU C 306	2.873 38.521 108.031 1.00 88.30	N
ATOM	3842 CA LEU C 306	1.813 38.932 107.102 1.00 87.75	С
	3843 C LEU C 306		С
ATOM	3844 O LEU C 306	1.494 37.623 105.105 1.00 86.96	О
ATOM	3845 CB LEU C 306	1.643 40.449 107.031 1.00 87.75	С
ATOM	3849 N ALA C 307	3.428 38.710 105.287 1.00 84.48	N
		3.975 38.243 104.036 1.00 83.02	С
		3.456 36.855 103.710 1.00 81.72	С
		2.787 36.700 102.691 1.00 81.74	Ο
ATOM	3853 CB ALA C 307	5.499 38.153 104.101 1.00 83.87	С
		3.741 35.897 104.578 1.00 80.64	N
ATOM		3.313 34.528 104.349 1.00 80.56	С
ATOM	3856 C LEU C 308	1.837 34.227 104.393 1.00 80.32	C
		1.451 33.090 104.129 1.00 81.28	0
		4.088 33.638 105.326 1.00 80.74	C
ATOM	3859 CG LEU C 308	5.606 33.702 105.214 1.00 81.07	С
ATOM	3860 CD1 LEU C 308	6.233 32.474 105.868 1.00 81.84	C
		6.072 33.806 103.771 1.00 81.43	N
	3862 N SER C 309	0.941 35.134 104.672 1.00 79.89 -0.479 34.948 104.731 1.00 79.30	C
		-1.221 35.614 103.592 1.00 78.26	c
	3864 C SER C 309 3865 O SER C 309	-2.261 35.090 103.204 1.00 79.47	O
	3866 CB SER C 309	-1.002 35.662 105.998 1.00 80.60	C
	3867 OG SER C 309	-0.215 35.163 107.066 1.00 83.66	Ö
	3868 N LEU C 310	-0.756 36.759 103.112 1.00 76.19	N
	3869 CA LEU C 310	-1.508 37.420 102.054 1.00 73.82	C
	3870 C LEU C 310	-1.655 36.484 100.863 1.00 73.16	Č
	3871 O LEU C 310	-0.922 35.521 100.655 1.00 73.48	Ö
	3872 CB LEU C 310	-0.896 38.740 101.649 1.00 73.31	Ċ
	3873 CG LEU C 310	-0.133 39.482 102.740 1.00 72.27	Č
	3874 CD1 LEU C 310	1.312 39.565 102.299 1.00 72.68	С
	3875 CD2 LEU C 310	-0.738 40.847 102.927 1.00 72.89	· C
	3876 N THR C 311	-2.687 36.805 100.099 1.00 71.77	N
	 		

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ATOM	3877 CA THR C 311	-2.995 36.006 98.906 1.00 70.70	С
ATOM		-2.290 36.693 97.760 1.00 69.86	C
		-2.027 37.901 97.909 1.00 69.35	0
ATOM	3880 CB THR C 311	-4.525 35.958 98.804 1.00 70.54	C
ATOM	3881 OG1 THR C 311	-5.119 37.248 98.625 1.00 70.13	0
		-5.108 35.381 100.078 1.00 69.62	C
		-2.027 36.051 96.633 1.00 69.24	N
ATOM	3884 CA ALA C 312	-1.352 36.731 95.535 1.00 69.20	C
		-1.994 38.096 95.309 1.00 70.12	C
		-1.276 39.088 95.102 1.00 69.29	0
		-1.319 35.905 94.278 1.00 68.74	C
		-3.336 38.147 95.357 1.00 71.47	N
ATOM	3889 CA ASP C 313	-3.987 39.441 95.163 1.00 72.61	С
		-3.647 40.479 96.208 1.00 70.88	С
ATOM	3891 O ASP C 313	-3.370 41.605 95.797 1.00 70.30	0
		-5.493 39.237 95.037 1.00 76.00	С
ATOM	3893 CG ASP C 313	-5.719 38.770 93.609 1.00 79.09	C ·
ATOM	3894 OD1 ASP C 313	-5.291 39.457 92.663 1.00 80.25	0
ATOM	3895 OD2 ASP C 313	-6.310 37.698 93.443 1.00 81.73	0
ATOM	3896 N GLN C 314	-3.619 40.161 97.488 1.00 69.54	N
ATOM	3897 CA GLN C 314	-3.275 41.129 98.517 1.00 69.05	С
		-1.827 41.588 98.406 1.00 67.22	С
ATOM	3899 O GLN C 314	-1.555 42.776 98.566 1.00 67.37	0
ATOM	3900 CB GLN C 314	-3.461 40.533 99.904 1.00 71.68 -4.663 39.606 99.946 1.00 73.75	C .
ATOM	3901 CG GLN C 314	-4.663 39.606 99.946 1.00 73.75	С
ATOM	3902 CD GLN C 314	-4.941 39.149 101.358 1.00 75.13	С
		-4.588 38.039 101.724 1.00 76.64	0
		-5.561 40.049 102.105 1.00 75.55	N
	3905 N MET C 315		N
		0.470 40.910 97.899 1.00 60.68	C
ATOM			C
	3908 O MET C 315	1.238 43.010 96.977 1.00 55.57	0
	3909 CB MET C 315	1.140 39.614 97.448 1.00 61.06	C
	3910 CG MET C 315	2.650 39.635 97.262 1.00 61.75	C
	3911 SD MET C 315	3.583 39.449 98.818 1.00 60.96	S
	3912 CE MET C 315	4.383 41.044 98.814 1.00 61.10	C
	3913 N VAL C 316	0.044 41.766 95.642 1.00 56.70	N
•	3914 CA VAL C 316	0.158 42.714 94.558 1.00 57.51	C
	3915 C VAL C 316	-0.261 44.121 94.967 1.00 59.23 0.397 45.117 94.654 1.00 59.22	C O
	3916 O VAL C 316		C
	3917 CB VAL C 316	-0.679 42.341 93.326 1.00 56.92 -0.569 43.429 92.272 1.00 56.72	C
	3918 CG1 VAL C 316 3919 CG2 VAL C 316	-0.569 43.429 92.272 1.00 56.72 -0.201 41.056 92.696 1.00 57.50	C
	3920 N SER C 317	-1.408 44.225 95.634 1.00 60.46	N
	3921 CA SER C 317	-1.408 44.223 93.834 1.00 60.40	C
A I OIVI	3921 CA SER C 317	1.00 00.01	C

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ATOM	4012	CA SER C 329	14.325 67.186 88.873 1.00 68.05	С
ATOM	4013	C SER C 329	14.324 68.663 89.244 1.00 70.45	С
ATOM	4014	O SER C 329	13.443 69.380 88.808 1.00 69.41	0
ATOM			15.044 67.000 87.545 1.00 66.88	C
			16.260 67.726 87.721 1.00 67.32	0
			15.292 69.079 90.029 1.00 75.28	N
			15.486 70.451 90.466 1.00 79.72	С
			15.752 71.335 89.247 1.00 80.73	С
			16.490 71.033 88.312 1.00 81.64	Ο
ATOM	4021	CB GLU C 330	16.659 70.570 91.435 1.00 83.87	С
ATOM	4022	CG GLU C 330	17.883 71.352 90.984 1.00 88.78	С
			19.152 70.582 90.643 1.00 91.78	С
			19.923 70.181 91.569 1.00 93.23	О
ATOM	4025	OE2 GLU C 330	19.404 70.377 89.422 1.00 92.87	0
			24.571 71.818 80.367 1.00 86.34	N
ATOM	4027	CA PHE C 337	24.988 70.495 80.814 1.00 85.91	C
			26.498 70.301 80.720 1.00 84.19	С
			27.064 70.525 79.646 1.00 85.85	О
ATOM	4030	CB PHE C 337	24.383 69.350 79.978 1.00 87.18	С
			23.005 68.970 80.445 1.00 88.47	С
			22.650 69.084 81.778 1.00 88.68	С
ATOM	4033	CD2 PHE C 337	22.068 68.507 79.534 1.00 89.03	С
ATOM	4034	CE1 PHE C 337	21.379 68.746 82.187 1.00 89.31	С
ATOM	4035	CE2 PHE C 337	20.795 68.160 79.942 1.00 89.22	С
			20.454 68.283 81.275 1.00 89.44	С
			27.095 69.868 81.803 1.00 80.55	N
			28.533 69.626 81.747 1.00 77.95	С
ATOM			28.746 68.395 82.598 1.00 76.21	С
ATOM			27.886 68.188 83.475 1.00 75.98	0
			29.228 70.829 82.347 1.00 78.52	C
			28.558 71.186 83.554 1.00 78.56	0
			29.821 67.656 82.395 1.00 73.78	N
			30.025 66.490 83.270 1.00 72.51	C
		C GLU C 339	29.556 66.874 84.677 1.00 71.03	C
		O GLU C 339	28.611 66.294 85.215 1.00 71.03	0
		CB GLU C 339	31.473 66.090 83.172 1.00 72.67	C
		CG GLU C 339	32.133 65.356 84.319 1.00 73.25	C
		CD GLU C 339	33.182 64.454 83.684 1.00 74.49	C
		OE1 GLU C 339	32.762 63.725 82.754 1.00 74.89	0
		OE2 GLU C 339	34.357 64.515 84.104 1.00 75.34	0
		N ALA C 340	30.147 67.886 85.304 1.00 68.89	N
		CA ALA C 340	29.747 68.302 86.619 1.00 67.05	C
		C ALA C 340	28.288 68.694 86.720 1.00 66.84	C
		O ALA C 340	27.647 68.263 87.697 1.00 68.55	0
ATOM	4056	CB ALA C 340	30.586 69.468 87.090 1.00 67.09	С

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			201/371	
ATOM	4102	O THR C 347	21.850 62.428 93.704 1.00 47.00	0
		CB THR C 347	24.621 62.957 91.764 1.00 46.71	С
		OG1 THR C 347	25.412 61.774 91.987 1.00 47.34	0
ATOM	4105	CG2 THR C 347	24.855 64.108 92.685 1.00 45.43	С
ATOM		N ASN C 348	21.741 64.272 92.536 1.00 48.38	N
ATOM	4107	CA ASN C 348	20.800 64.933 93.432 1.00 48.80	С
ATOM	4108	C ASN C 348	19.478 64.160 93.443 1.00 47.26	С
ATOM	4109	O ASN C 348	18.850 63.828 94.448 1.00 46.97	Ο
ATOM	4110	CB ASN C 348	20.589 66.367 92.932 1.00 51.67	С
ATOM	4111	CG ASN C 348	19.510 67.096 93.727 1.00 55.80	С
		OD1 ASN C 348	18.292 67.162 93.409 1.00 56.91	0
ATOM	4113	ND2 ASN C 348	20.009 67.668 94.842 1.00 56.64	N
		N LEU C 349	18.996 63.846 92.246 1.00 45.48	N
		CA LEU C 349	17.730 63.135 92.094 1.00 43.91	С
		C LEU C 349	17.843 61.824 92.848 1.00 42.97	C
		O LEU C 349	16.938 61.492 93.603 1.00 42.67	0
		CB LEUC 349	17.402 63.025 90.592 1.00 44.22	C
		CG LEU C 349	16.113 62.256 90.280 1.00 45.28	C
ATOM		CD1 LEU C 349	14.890 63.005 90.815 1.00 44.98	C
		CD2 LEU C 349	15.924 61.981 88.802 1.00 45.98	C
		N ALA C 350	18.925 61.069 92.685 1.00 42.54	N
		CA ALA C 350	19.170 59.789 93.329 1.00 41.93	C
		C ALA C 350	19.145 59.965 94.846 1.00 42.66	C
		O ALA C 350	18.382 59.288 95.534 1.00 42.32	O C
		CB ALA C 350	20.519 59.214 92.915 1.00 41.05 19.924 60.909 95.377 1.00 42.85	N
ATOM		N ASP C 351	19.891 61.156 96.801 1.00 44.92	C
ATOM		CA ASP C 351 C ASP C 351	18.473 61.409 97.333 1.00 46.20	c
-		O ASP C 351		0
			20.806 62.330 97.121 1.00 47.28	C
			20.808 62.552 98.629 1.00 49.76	Č
		OD1 ASP C 351	21.507 61.847 99.383 1.00 49.99	o
		OD2 ASP C 351	20.076 63.475 99.055 1.00 51.97	Ö
		N ARG C 352	17.580 62.055 96.578 1.00 45.35	N
		CA ARG C 352	16.230 62.286 97.039 1.00 44.90	C
		C ARG C 352	15.377 61.039 96.994 1.00 45.67	С
		O ARG C 352	14.604 60.740 97.920 1.00 46.34	Ο
		CB ARG C 352	15.622 63.384 96.190 1.00 45.66	С
ATOM	4140	CG ARG C 352	16.211 64.727 96.599 1.00 47.97	С
ATOM	4141	CD ARG C 352	15.095 65.784 96.368 1.00 49.73	С
ATOM	4142	NE ARG C 352	15.270 66.120 94.954 1.00 51.59	N
ATOM	4143	CZ ARG C 352	14.259 66.180 94.076 1.00 52.43	С
ATOM	4144	NH1 ARG C 352	13.012 65.962 94.496 1.00 50.90	N
ATOM	4145	NH2 ARG C 352	14.668 66.482 92.828 1.00 52.24	N
ATOM	4146	N GLU C 353	15.480 60.234 95.928 1.00 45.42	N

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			202/371	
ATOM	4147	CA GLU C 353	14.681 59.005 95.829 1.00 44.09	С
ATOM		C GLU C 353	15.048 57.996 96.931 1.00 43.54	С
ATOM	4149			Ο
ATOM	4150	CB GLU C 353	14.925 58.352 94.479 1.00 43.55	С
ATOM		CG GLU C 353	14.829 59.283 93.288 1.00 44.01	С
ATOM	4152	CD GLU C 353	14.774 58.522 91.971 1.00 44.71	С
ATOM	4153	OE1 GLU C 353	13.863 57.703 91.769 1.00 44.74	О
ATOM	4154	OE2 GLU C 353	15.652 58.718 91.111 1.00 45.16	0
ATOM		N LEU C 354	16.297 58.121 97.413 1.00 42.25	N
ATOM		CA LEU C 354	16.817 57.236 98.424 1.00 42.36	С
ATOM			15.967 57.327 99.669 1.00 43.23	С
ATOM			15.622 56.324 100.303 1.00 44.20	0
ATOM		CB LEU C 354		C
		CG LEU C 354	19.142 56.685 97.709 1.00 41.03	C
		CD1 LEU C 354	20.499 57.306 97.552 1.00 41.57	C
		CD2 LEU C 354	19.154 55.273 98.236 1.00 41.51	C
		N VAL C 355		N
ATOM		CA VAL C 355	14.766 58.766 101.172 1.00 43.54	C
ATOM		C VAL C 355		C
ATOM		O VAL C 355		O C
			14.536 60.278 101.340 1.00 42.48 13.633 60.512 102.513 1.00 42.64	(
		CG1 VAL C 355	15.872 60.974 101.564 1.00 42.45	
		CG2 VAL C 355 N HIS C 356	12.773 58.241 99.854 1.00 44.10	N
ATOM ATOM			11.514 57.552 99.623 1.00 45.02	C
ATOM		C HIS C 356	11.760 56.068 99.613 1.00 44.50	C
ATOM	4173		10.931 55.306 100.111 1.00 44.42	0
ATOM		-	10.881 58.057 98.313 1.00 48.88	Č
-		CG HIS C 356	10.545 59.504 98.508 1.00 51.53	C
			9.269 59.940 98.714 1.00 52.82	N
		CD2 HIS C 356		С
		CE1 HIS C 356	9.287 61.255 98.886 1.00 53.87	С
		NE2 HIS C 356	10.534 61.686 98.805 1.00 54.36	N
		N MET C 357	12.893 55.662 99.024 1.00 44.54	N
ATOM	4181	CA MET C 357	13.210 54.233 98.928 1.00 43.62	C
ATOM	4182	C MET C 357	13.141 53.532 100.274 1.00 42.21	С
ATOM	4183	O MET C 357	12.466 52.525 100.393 1.00 42.85	О
		CB MET C 357	14.574 53.907 98.327 1.00 43.25	C
		CG MET C 357	14.636 52.406 97.985 1.00 42.60	C
		SD MET C 357	16.349 52.075 97.453 1.00 42.35	S
		CE MET C 357	16.261 52.824 95.831 1.00 43.46	C
		N ILE C 358	13.834 54.096 101.243 1.00 40.42	N
		CA ILE C 358	13.815 53.539 102.582 1.00 39.96	C
		C ILE C 358	12.394 53.337 103.074 1.00 41.38	C
ATOM	4191	O ILE C 358	12.056 52.287 103.607 1.00 41.84	О

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ATOM	4192	CB ILE C 358	14.587 54.473 103.522 1.00 37.30	С
		CG1 ILE C 358	16.020 54.488 103.073 1.00 37.04	С
ATOM		CG2 ILE C 358	14,503 54,006 104,933 1.00 37.30	С
ATOM		CD1 ILE C 358	16,901 55,392 103,869 1.00 38,43	С
ATOM	4196	N ASN C 359	11.533 54.324 102.909 1.00 43.86	N
ATOM	4197	CA ASN C 359	10.146 54.230 103.335 1.00 46.73	С
ATOM	4198	C ASN C 359	9.476 53.068 102.650 1.00 46.07	Ċ
ATOM	4199	O ASN C 359	8.928 52.164 103.263 1.00 47.05	
ATOM		CB ASN C 359	9.407 55.532 103.002 1.00 52.10	С
		CG ASN C 359	9.815 56.559 104.061 1.00 57.06	C
		OD1 ASN C 359	9.530 56.230 105.237 1.00 61.37	0
		ND2 ASN C 359	10.443 57.691 103.772 1.00 57.61	N
		N TRP C 360	9.568 53.055 101.326 1.00 44.98	N
		CA TRP C 360	8.980 51.992 100.530 1.00 43.27	C
		C TRP C 360	9.436 50.637 101.030 1.00 43.73	C O
		O TRP C 360 CB TRP C 360	8.653 49.706 101.171 1.00 44.79 9.485 52.208 99.101 1.00 42.81	C
		CG TRP C 360	9,293 50,969 98.261 1.00 43.02	C
ATOM		CD1 TRP C 360	8.121 50.582 97.690 1.00 42.68	C
		CD2 TRP C 360	10.270 49.978 97.909 1.00 42.05	C
		NE1 TRP C 360	8.335 49.411 97.017 1.00 43.15	N
		CE2 TRP C 360	9,632 49.020 97.128 1.00 42.10	C
		CE3 TRP C 360	11.619 49.812 98.190 1.00 42.67	С
		CZ2 TRP C 360	10.261 47.902 96.606 1.00 42.59	C
		CZ3 TRP C 360	12.278 48.711 97.685 1.00 43.71	С
ATOM		CH2 TRP C 360	11.598 47.767 96.899 1.00 43.79	С
ATOM	4218	N ALA C 361	10.732 50.463 101.287 1.00 43.63	N
ATOM	4219	CA ALA C 361	11.262 49.197 101.739 1.00 44.41	С
		C ALA C 361	10.474 48.726 102.959 1.00 46.03	С
			10.110 47.541 103.017 1.00 45.76	0
		=	12.745 49.292 102.036 1.00 43.71	C
		N LYS C 362	10.182 49.624 103.894 1.00 47.55	. N
		CA LYS C 362	9.463 49.250 105.089 1.00 50.72	C
		C LYS C 362	8.117 48.616 104.849 1.00 51.32	C
		O LYS C 362	7.705 47.864 105.734 1.00 52.47 9.354 50.432 106.038 1.00 53.23	C
		CB LYS C 362	10.720 50.832 106.594 1.00 56.10	C
		CG LYS C 362 CD LYS C 362	11.155 49.773 107.599 1.00 60.05	Č
		CE LYS C 362	11.762 50.371 108.869 1.00 62.37	C
		NZ LYS C 362	11.973 49.344 109.950 1.00 63.33	N
		N ARG C 363	7.456 48.823 103.745 1.00 51.32	N
		CA ARG C 363	6.186 48.226 103.427 1.00 52.74	C
		C ARG C 363	6.288 47.007 102.539 1.00 51.87	C
		O ARG C 363	5.238 46.502 102.129 1.00 53.22	0
		CB ARG C 363	5.351 49.253 102.657 1.00 56.62	С
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ATOM	4237	CG ARG C 363	6.006 50.631 102.784 1.00 62.69	С
ATOM	4238	CD ARG C 363	5.368 51.299 104.018 1.00 68.16	С
ATOM	4239	NE ARG C 363	3.954 51.463 103.640 1.00 73.89	N
ATOM	4240	CZ ARG C 363	3.622 52.373 102.697 1.00 77.79	С
ATOM	4241	NH1 ARG C 363	4.613 53.120 102.163 1.00 78.54	N
ATOM		NH2 ARG C 363	2.326 52.501 102.337 1.00 78.75	N
ATOM		N VAL C 364	7.443 46.512 102.137 1.00 50.42	N
ATOM		CA VAL C 364	7.407 45.312 101.264 1.00 48.81	С
ATOM		C VAL C 364	7.152 44.136 102.175 1.00 48.62	C
ATOM		O VAL C 364	7.960 43.818 103.056 1.00 49.16	0
ATOM		CB VAL C 364	8.758 45.196 100.552 1.00 47.54	C
ATOM		CG1 VAL C 364	8.932 43.867 99.857 1.00 46.99	C C
ATOM		CG2 VAL C 364	8.826 46.340 99.567 1.00 47.58	· N
ATOM		N PRO C 365	6.032 43.475 102.044 1.00 48.21 5.681 42.339 102.907 1.00 48.44	C
ATOM		CA PRO C 365 C PRO C 365	6.876 41.471 103.242 1.00 48.67	c
ATOM		O PRO C 365	7.614 41.066 102.349 1.00 49.90	O
ATOM ATOM		CB PRO C 365	4.552 41.591 102.187 1.00 47.40	C
ATOM		CG PRO C 365	3.903 '42.813 101.550 1.00 48.29	Č
ATOM		CD PRO C 365	5.000 43.764 101.059 1.00 47.57	č
ATOM		N GLY C 366	7.125 41.223 104.524 1.00 48.37	N
ATOM		CA GLY C 366	8.198 40.394 105.005 1.00 47.61	C
ATOM		C GLY C 366	9.486 41.099 105.359 1.00 47.49	С
ATOM	4260		10.295 40.559 106.123 1.00 48.03	Ο
ATOM	4261	N PHE C 367	9.712 42.282 104.809 1.00 46.58	N
ATOM	4262	CA PHE C 367	10.945 43.027 105.006 1.00 45.91	С
ATOM	4263	C PHE C 367	11.205 43.352 106.462 1.00 46.07	С
ATOM		O PHE C 367	12.240 43.121 107.078 1.00 46.31	0
		CB PHE C 367		C
ATOM		CG PHE C 367	12.177 45.108 104.254 1.00 45.43	C
ATOM		CD1 PHE C 367	13.256 44.686 103.505 1.00 44.99	C
			12.322 46.248 105.045 1.00 45.56	C
		CE1 PHE C 367		C C
		CE2 PHE C 367		C
		CZ PHE C 367	14.587 46.507 104.302 1.00 44.85 10.183 43.916 107.063 1.00 46.69	N
		N VAL C 368 CA VAL C 368	10.167 44.342 108.456 1.00 48.15	Ċ
		C VAL C 368	10.370 43.209 109.433 1.00 49.45	c
		O VAL C 368	10.729 43.461 110.576 1.00 51.13	Ö
		CB VAL C 368	8.839 45.093 108.697 1.00 47.28	č
		CG1 VAL C 368	8.130 44.630 109.922 1.00 46.30	C
		CG2 VAL C 368	9.166 46.584 108.675 1.00 47.60	Ċ
		N ASP C 369	10.179 41.953 109.060 1.00 49.63	N
		CA ASP C 369	10.429 40.828 109.904 1.00 49.20	С
ATOM		C ASP C 369	11.912 40.582 110.004 1.00 47.87	С
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ATOM	4282	O ASP C 369	12.265 39.674 110.747 1.00 50.06	0
ATOM		CB ASP C 369	9.807 39.560 109.326 1.00 52.94	С
ATOM		CG ASP C 369	8.306 39.646 109.140 1.00 57.07	С
ATOM	4285	OD1 ASP C 369	7.536 40.253 109.942 1.00 58.15	Ο
ATOM	4286	OD2 ASP C 369	7.883 39.050 108.107 1.00 59.37	Ο
ATOM	4287	N LEU C 370	12.821 41.214 109.311 1.00 46.81	N
ATOM		CA LEU C 370	14.258 40.966 109.428 1.00 45.04	С
ATOM	-	C LEU C 370	14.866 41.839 110.513 1.00 43.57	C
ATOM		O LEU C 370	14.254 42.837 110.910 1.00 43.75	0
ATOM		CB LEUC 370	14.890 41.285 108.071 1.00 45.57	C
ATOM		CG LEU C 370	14.408 40.389 106.933 1.00 45.97	C
ATOM		CD1 LEU C 370	15.101 40.776 105.637 1.00 46.19	C
ATOM		CD2 LEU C 370	14.724 38.931 107.276 1.00 45.91	C
ATOM		N THR C 371	16.039 41.536 111.036 1.00 42.53	N C
ATOM		CA THR C 371	16.580 42.386 112.100 1.00 41.92 16.872 43.746 111.509 1.00 42.67	C
ATOM		C THR C 371 O THR C 371	17.204 43.891 110.332 1.00 43.23	Ö
ATOM ATOM	4298	O THR C 371 CB THR C 371	17.873 41.796 112.640 1.00 42.10	C
ATOM		OG1 THR C 371	18.638 41.467 111.456 1.00 43.55	o
ATOM		CG2 THR C 371	17.637 40.557 113.466 1.00 41.52	Č
ATOM		N LEUC 372	16,806 44,784 112,334 1.00 43.35	N
ATOM		CA LEU C 372	17.071 46.123 111.810 1.00 43.84	С
ATOM		C LEUC 372	18.357 46.185 111.004 1.00 44.86	C
ATOM		O LEU C 372	18.366 46.867 109.970 1.00 44.98	. 0
ATOM	4306	CB LEU C 372	17.024 47.102 112.965 1.00 42.98	С
ATOM	4307	CG LEU C 372	15.695 47.307 113.677 1.00 41.37	, C
ATOM		CD1 LEU C 372	15.874 48.209 114.886 1.00 41.90	С
ATOM		CD2 LEU C 372	14.703 47.968 112.755 1.00 40.39	С
ATOM		N HIS C 373	19.435 45.513 111.409 1.00 45.75	N
ATOM		CA HIS C 373	20.661 45.607 110.630 1.00 47.06	С
ATOM		C HIS C 373	20.502 44.905 109.308 1.00 46.38	C
		O HIS C 373	21.005 45.465 108.331 1.00 45.68	0
		CB HIS C 373	21.832 45.143 111.475 1.00 50.24	C
		CG HIS C 373	22.249 46.192 112.465 1.00 52.68 21.884 46.194 113.800 1.00 53.78	N
		ND1 HIS C 373	22.999 47.288 112.334 1.00 53.37	C
		CD2 HIS C 373 CE1 HIS C 373	22.421 47.255 114.401 1.00 54.11	Č
		NE2 HIS C 373	23.112 47.959 113.519 1.00 54.30	N
		N ASP C 374	19.792 43.778 109.258 1.00 45.87	N
		CA ASP C 374	19.599 43.113 107.963 1.00 45.03	С
		C ASP C 374	18.832 43.997 107.004 1.00 44.25	C
		O ASP C 374	19.180 44.045 105.812 1.00 44.05	Ο
		CB ASP C 374	18.986 41.731 108.142 1.00 46.40	C
		CG ASP C 374	20.139 40.886 108.665 1.00 48.80	С
		OD1 ASP C 374	21.283 41.356 108.487 1.00 49.03	О

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ATOM	4462	N LEU C 391	14.058 53.497 86.851 1.00 42.39	N
ATOM		CA LEU C 391	14.309 54.343 85.679 1.00 42.48	С
ATOM		C LEU C 391	13.889 53.586 84.434 1.00 43.75	С
ATOM		O LEU C 391	13.060 54.004 83.635 1.00 44.31	Ο
ATOM		CB LEU C 391	15.790 54.665 85.609 1.00 42.32	C
ATOM	4467	CG LEU C 391	16.325 55.261 84.318 1.00 42.43	С
ATOM	4468	CD1 LEU C 391	15.626 56.583 84.058 1.00 42.19	С
ATOM	4469	CD2 LEU C 391	17.840 55.475 84.358 1.00 42.78	С
ATOM	4470	N VAL C 392	14.451 52.387 84.261 1.00 44.61	N
ATOM	4471	CA VAL C 392	14.127 51.568 83.101 1.00 45.11	С
ATOM		C VAL C 392	12.622 51.507 82.873 1.00 46.00	С
ATOM		O VAL C 392		0
ATOM		CB VAL C 392		С
ATOM		CG1 VAL C 392	14.210 49.215 82.193 1.00 43.32	C
ATOM		CG2 VAL C 392	16.262 50.250 82.999 1.00 42.75	C
		N TRP C 393	11.902 51.174 83.924 1.00 46.93	N
		CA TRP C 393	10.453 51.019 83.882 1.00 48.43	C
		C TRP C 393	9.711 52.279 83.483 1.00 48.79	C
ATOM				0
ATOM			9.937 50.621 85.262 1.00 48.30	C C
ATOM		CG TRP C 393	8.481 50.845 85.442 1.00 48.18 7.912 51.799 86.217 1.00 49.07	C
ATOM		CD1 TRP C 393 CD2 TRP C 393	7.408 50.122 84.849 1.00 48.75	C
ATOM		NE1 TRP C 393	6.537 51.695 86.155 1.00 49.00	N
		CE2 TRP C 393	6.206 50.675 85.324 1.00 48.09	C
		CE3 TRP C 393	7.349 49.030 83.968 1.00 49.78	č
ATOM		CZ2 TRP C 393		Č
ATOM		CZ3 TRP C 393	6.099 48.547 83.591 1.00 49.68	Č
ATOM		CH2 TRP C 393	4.928 49.138 84.089 1.00 49.25	C
		N ARG C 394		N
ATOM		CA ARG C 394	9.450 54.634 83.700 1.00 47.92	С
ATOM	4493	C ARG C 394	9.934 55.088 82.344 1.00 49.43	С
ATOM	4494	O ARG C 394	9.287 55.925 81.730 1.00 51.46	Ο
ATOM	4495	CB ARG C 394	9.503 55.746 84.710 1.00 46.47	С
ATOM	4496	CG ARG C 394	10.763 56.081 85.415 1.00 45.70	С
ATOM	4497	CD ARG C 394	10.566 57.207 86.424 1.00 44.60	С
		NE ARG C 394	11.920 57.710 86.742 1.00 44.81	N
		CZ ARG C 394	12.693 57.162 87.681 1.00 43.57	С
		NH1 ARG C 394	12.145 56.129 88.322 1.00 43.13	N
		NH2 ARG C 394	13.896 57.673 87.883 1.00 41.36	N
ATOM			11.021 54.572 81.810 1.00 51.47	N
		CA SER C 395	11.529 55.002 80.516 1.00 51.90	C
		C SER C 395	10.991 54.173 79.388 1.00 53.62	С
ATOM			11.334 54.434 78.247 1.00 54.61	O C
AIUM	4506	CB SEK C 395	13.065 54.848 80.552 1.00 50.43	C

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ΛΤΩΝ	4507 OG SER C 305	13.612 55.991 81.184 1.00 48.96	0
ATOM	4507 OG SER C 393	10.218 53.150 79.665 1.00 56.89	N
ATOM	4509 CA MET C 396	9.697 52.238 78.670 1.00 60.23	C
ATOM	4510 C MET C 396	9.095 52.842 77.413 1.00 63.30	c
		9.523 52.504 76.297 1.00 63.66	
ATOM	4512 CB MET C 396	8,583 51,406 79,298 1,00 59,55	С
ATOM	4513 CG MET C 396	8.583 51.406 79.298 1.00 59.55 8.723 49.930 79.002 1.00 59.80	С
ATOM	4514 SD MET C 396	7.886 49.083 80.359 1.00 61.85	S
ATOM	4515 CE MET C 396	6.596 48.204 79.499 1.00 61.89	С
ATOM	4516 N GLU C 397	8.110 53.729 77.604 1.00 66.03	N
ATOM	4517 CA GLU C 397	7.439 54.322 76.470 1.00 69.27	С
		8.151 55.504 75.901 1.00 67.82	
ATOM	4519 O GLUC 397	7.474 56.429 75.435 1.00 69.29	0
ATOM	4520 CB GLU C 397	6.018 54.786 76.785 1.00 74.53 5.187 53.758 77.541 1.00 81.19	C C
ATOM	4521 CG GLU C 397	5.187 53.758 77.541 1.00 81.19	C
ATOM	4322 CD GLU C 397	5.613 53.797 79.002 1.00 85.34 6.269 54.817 79.359 1.00 86.81	0
ATOM	4524 OF2 GULC 397	5.316 52.820 79.737 1.00 88.67	
ATOM	4525 N HIS C 398	9.452 55.666 75.936 1.00 65.73	N
		10.154 56.801 75.368 1.00 64.19	
		11.390 56.162 74.750 1.00 63.33	
ATOM	4528 O HIS C 398	12.489 56.333 75.265 1.00 64.80	0
ATOM	4529 CB HIS C 398	10.584 57.864 76.359 1.00 65.69	С
ATOM	4530 CG HIS C 398	9.454 58.536 77.071 1.00 67.75	\mathbf{C}
		8.465 57.788 77.699 1.00 68.11	
ATOM	4532 CD2 HIS C 398	9.121 59.824 77.286 1.00 68.37	С
ATOM	4533 CEI HIS C 398	7.559 58.547 78.254 1.00 68.33 7.943 59.791 78.021 1.00 69.24	C
ATOM	4534 NE2 HIS C 398	7.943 59.791 78.021 1.00 69.24	IN NI
		11.169 55.409 73.695 1.00 61.57 12.201 54.677 72.989 1.00 60.18	
		13.406 55.548 72.785 1.00 59.34	
	4538 O PRO C 399	13.227 56.719 72.471 1.00 60.76	Ö
	4539 CB PRO C 399	11.624 54.256 71.635 1.00 60.20	C
	4540 CG PRO C 399	10.177 54.105 72.045 1.00 61.13	С
	4541 CD PRO C 399	9.883 55.172 73.063 1.00 61.15	C ·
	4542 N GLY C 400	14.584 55.028 73.029 1.00 58.02	N
	4543 CA GLY C 400	15.779 55.810 72.817 1.00 57.60	С
	4544 C GLY C 400	16.055 56.848 73.866 1.00 57.41	C
	4545 O GLY C 400	17.142 57.465 73.774 1.00 59.48	0
	4546 N LYS C 401	15.168 57.029 74.824 1.00 55.91	N
	4547 CA LYS C 401	15.375 58.004 75.873 1.00 56.17	C C
	4548 C LYS C 401 4549 O LYS C 401	15.214 57.440 77.288 1.00 54.71 14.614 56.395 77.534 1.00 53.87	0
	4550 CB LYS C 401	14.325 59.092 75.773 1.00 58.67	C
	4551 CG LYS C 401		Č
711 OW	,551 CC D16 C 401	15.505 55.055 77,715 1.00 01.01	•

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	4642 CZ ARG C 412		C
	4643 NH1 ARG C 412	25.379 56.961 71.564 1.00 68.04	N N
ATOM	4644 NH2 ARG C 412	26.531 55.145 72.370 1.00 67.64 22.590 60.264 73.461 1.00 67.18	N
ATOM	4645 N ASN C 413	23.727 61.134 73.215 1.00 69.57	C
ATOM	4647 C ASN C 413	24.062 62.069 74.338 1.00 68.89	c
ATOM	4648 O ASN C 413	25.249 62.371 74.517 1.00 69.37	Ö
ATOM	4649 CB ASN C 413	23.457 61.894 71.902 1.00 73.23	С
ATOM	4650 CG ASN C 413	23.211 60.796 70.856 1.00 76.66	С
ATOM	4651 OD1 ASN C 413	24.175 60.090 70.514 1.00 77.59	Ο
ATOM	4652 ND2 ASN C 413	21.937 60.700 70.451 1.00 78.09	N
ATOM	4653 N GLN C 414	23.126 62.512 75.161 1.00 67.79	N
ATOM	4654 CA GLN C 414	23.439 63.399 76.274 1.00 67.35	C
ATOM	4655 C GLN C 414	24.282 62.671 77.308 1.00 67.26	C
ATOM	4656 O GLN C 414	24,986 63.252 78.133 1.00 66.80	0
ATOM	4657 CB GLN C 414	22.170 63.973 76.860 1.00 68.30	C C
ATOM	4658 CG GLN C 414	21.127 64.314 75.798 1.00 69.45 20.117 65.274 76.396 1.00 70.67	C
	4660 OE1 GLN C 414	18.908 65.040 76.412 1.00 71.62	Ō
	4661 NE2 GLN C 414		N
ATOM	4662 N GLY C 415	24.280 61.344 77.244 1.00 67.32	N
ATOM	4663 CA GLY C 415	25.114 60.498 78.069 1.00 67.57	С
ATOM	4664 C GLY C 415	26.543 60.925 77.798 1.00 67.85	С
ATOM	4665 O GLY C 415	27.295 61.154 78.738 1.00 68.28	0
ATOM	4666 N LYS C 416	26.974 61.147 76.566 1.00 69.42	N
		28.343 61.564 76.260 1.00 70.20	C
ATOM	4668 C LYS C 416	28.826 62.756 77.069 1.00 68.84	C
ATOM	4669 O LYS C 416	30.035 62.973 77.197 1.00 68.46	0
ATOM	4670 CB LYS C 416	28.536 61.814 74.774 1.00 72.02	C C
ATOM	4671 CG LYS C 416	27.801 60.834 73.887 1.00 75.13 28.735 60.255 72.828 1.00 78.53	C
	4673 CE LYS C 416	28.299 60.701 71.428 1.00 80.96	C
	4674 NZ LYS C 416	27.171 59.853 70.902 1.00 82.97	N
	4675 N CYS C 417	27.957 63.544 77.671 1.00 67.72	N
	4676 CA CYS C 417	28.400 64.669 78.473 1.00 68.04	С
	4677 C CYS C 417	29.289 64.173 79.591 1.00 65.78	С
	4678 O CYS C 417	30.319 64.804 79.839 1.00 66.63	0
ATOM	4679 CB CYS C 417	27.189 65.495 78.933 1.00 70.16	С
	4680 SG CYS C 417	26.344 66.190 77.467 1.00 75.80	S
	4681 N VAL C 418	28.954 63.094 80.279 1.00 63.41	N
	4682 CA VAL C 418	29.782 62.604 81.370 1.00 61.12	C
ATOM	4683 C VAL C 418	30.653 61.452 80.918 1.00 60.84	C
ATOM	4684 O VAL C 418	30.146 60.621 80.184 1.00 60.27	O C
	4685 CB VAL C 418	28.910 62.163 82.549 1.00 60.20 29.739 61.551 83.665 1.00 60.01	C
ATOM	4686 CG1 VAL C 418	23.735 01.331 03.003 1.00 00.01	C

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			28.137 63.359 83.076 1.00 59.97	C
ATOM	4688	N GLU C 419	31.894 61.419 81.335 1.00 62.11	N
ATOM	4689	CA GLU C 419	32.844 60.376 81.019 1.00 64.89	С
ATOM	4690	C GLU C 419	32.362 58.995 81.400 1.00 64.14	С
ATOM	4691	O GLU C 419	31.817 58.720 82.462 1.00 64.65	Ο
ATOM	4692	CB GLU C 419	34.097 60.663 81.830 1.00 69.95	С
ATOM	4693	CG GLU C 419	35.415 60.468 81.108 1.00 77.04	С
ATOM	4694	CD GLU C 419	36.572 60.336 82.092 1.00 82.02	C
ATOM	4695	OE1 GLU C 419	36.507 60.945 83.209 1.00 84.55	Ο
ATOM	4696	OE2 GLU C 419	37.561 59.616 81.759 1.00 84.42	0
ATOM	4697	N GLY C 420	32.489 58.009 80.543 1.00 63.83	N
ATOM	4698	CA GLY C 420	32.053 56.657 80.783 1.00 63.46	С
ATOM	4699	C GLY C 420	30.585 56.411 81.000 1.00 63.33	С
ATOM	4700	O GLY C 420	30.235 55.276 81.342 1.00 64.98	Ο
ATOM	4701	N MET C 421	29.655 57.314 80.838 1.00 62.92	N
ATOM	4702	CA MET C 421	28.242 57.162 81.035 1.00 61.73	C
ATOM	4703	C MET C 421	27.448 56.561 79.900 1.00 60.56	С
ATOM	4704	O MET C 421	26.393 55.981 80.122 1.00 60.92	0
ATOM	4705	CB MET C 421	27.639 58.571 81.229 1.00 62.59	С
ATOM	4706	CG MET C 421	27.591 58.918 82.704 1.00 64.61	С
ATOM	4707	SD MET C 421	25.913 58.610 83.314 1.00 67.20	S
ATOM	4708	CE MET C 421	25.173 60.208 82.895 1.00 66.86	С
			27.896 56.713 78.674 1.00 59.89	N
			27.177 56.240 77.518 1.00 59.46	C
		C VAL C 422		С
			25.812 54.359 77.160 1.00 58.65	Ο
			27.919 56.440 76.175 1.00 60.40	С
ATOM	4714	CG1 VAL C 422	26.932 56.991 75.156 1.00 61.42	С
		CG2 VAL C 422		C
			27.910 53.993 78.049 1.00 58.67	N
			27.762 52.547 78.109 1.00 58.29	С
		C GLU C 423		С
ATOM			25.911 51.254 78.862 1.00 56.05	0
		CB GLU C 423	29.023 51.835 78.541 1.00 62.43	С
		CG GLU C 423		С
		CD GLU C 423	30.915 53.376 78.163 1.00 72.99	С
		OE1 GLU C 423	30.415 54.513 78.012 1.00 74.11	0
		OE2 GLU C 423	32.004 53.165 78.762 1.00 76.42	0
		N ILE C 424	26.662 52.944 80.214 1.00 51.13	N
		CA ILE C 424	25.646 52.689 81.221 1.00 47.44	С
		C ILE C 424	24.324 53.032 80.585 1.00 47.25	C
		O ILE C 424	23.394 52.213 80.556 1.00 48.16	Ο
		CB ILE C 424	26.040 53.450 82.464 1.00 46.56	C
		CG1 ILE C 424	27.332 52.804 82.970 1.00 46.07	C
ATOM	473 1	CG2 ILE C 424	25.006 53.384 83.575 1.00 47.25	С

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ATOM 4776 N ALA C 430 18.796 49.343 76.515 1.00 42.18

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ATOM	4777 CA ALA C 430	18.544 47.963 76.137 1.00 42.04	С
ATOM		17.580 47.280 77.101 1.00 42.71	С
ATOM	4779 O ALA C 430	16.751 46.465 76.666 1.00 44.50	0
ATOM	4780 CB ALA C 430	19.866 47.211 76.195 1.00 42.17	С
	4781 N THR C 431	17.670 47.540 78.401 1.00 41.61	N
	4782 CA THR C 431	16.764 46.859 79.309 1.00 41.93	С
ATOM		15.378 47.412 79.090 1.00 42.69	С
ATOM	4784 O THR C 431	14.347 46.744 79.063 1.00 41.58	0
	4785 CB THR C 431	17.133 47.151 80.772 1.00 42.56	С
	4786 OG1 THR C 431	18.546 46.950 80.878 1.00 44.44	Ο
	4787 CG2 THR C 431	16.344 46.278 81.723 1.00 40.93	С
ATOM		15.404 48.745 78.942 1.00 45.20	N
	4789 CA SER C 432	14.149 49.490 78.767 1.00 46.82	С
	4790 C SER C 432	13.390 48.962 77.561 1.00 46.53	С
ATOM	4791 O SER C 432	12.191 48.710 77.540 1.00 46.14	Ο
ATOM	4792 CB SER C 432	14.392 50.986 78.698 1.00 47.74	С
ATOM	4793 OG SER C 432	13.074 51.509 78.440 1.00 50.00	О
ATOM	4794 N SER C 433	14.150 48.747 76.514 1.00 47.34	N
ATOM	4795 CA SER C 433	13.668 48.149 75.292 1.00 49.60	С
ATOM	4796 C SER C 433	13.123 46.748 75.472 1.00 49.87	С
ATOM	4797 O SER C 433	12.017 46.389 75.083 1.00 49.55	О
ATOM	4798 CB SER C 433	14.950 48.089 74.459 1.00 51.76	С
ATOM	4799 OG SER C 433	14.471 47.977 73.129 1.00 57.08	О
ATOM		13.863 45.867 76.147 1.00 51.89	N.
ATOM		13.411 44.512 76.446 1.00 53.04	C
	4802 C ARG C 434	12.110 44.574 77.248 1.00 53.63	C
ATOM		11.188 43.778 77.007 1.00 52.87	0
	4804 CB ARG C 434	14.457 43.666 77.163 1.00 53.71	C
	4805 CG ARG C 434	13.927 42.293 77.511 1.00 56.12	C
	4806 CD ARG C 434		C
	4807 NE ARG C 434	14.084 39.828 77.305 1.00 60.35	N
	4808 CZ ARG C 434	13.212 39.481 76.350 1.00 61.02	C
	4809 NH1 ARG C 434		N
	4810 NH2 ARG C 434		N
	4811 N PHE C 435	11.994 45.517 78.200 1.00 54.32	N
	4812 CA PHE C 435	10.747 45.613 78.954 1.00 55.85	C
	4813 C PHE C 435	9.604 45.980 78.009 1.00 57.99	C
	4814 O PHE C 435	8.488 45.463 78.148 1.00 57.42	0
	4815 CB PHE C 435	10.833 46.587 80.108 1.00 55.50	C
	4816 CG PHE C 435	11.450 46.066 81.373 1.00 55.59	C
	4817 CD1 PHE C 435	11.748 44.719 81.548 1.00 55.40	C
	4818 CD2 PHE C 435	11.735 46.941 82.410 1.00 54.85	C C
	4819 CE1 PHE C 435	12.330 44.252 82.692 1.00 54.88	C
	4820 CE2 PHE C 435	12.312 46.512 83.573 1.00 54.54	C
ATOM	4821 CZ PHE C 435	12.609 45.163 83.698 1.00 55.69	C

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ATOM	4822 N ARG C 436	9.895 46.864 77.039 1.00 60.12	N
		8.905 47.250 76.049 1.00 62.03	С
ATOM	4824 C ARG C 436	8.479 46.028 75.247 1.00 63.18	С
ATOM	4825 O ARG C 436	7.300 45.695 75.167 1.00 63.07	Ο
ATOM	4826 CB ARG C 436	9.489 48.295 75.126 1.00 63.26	С
ATOM	4827 CG ARG C 436	8.479 49.271 74.577 1.00 65.79	С
ATOM	4828 CD ARG C 436	9.088 50.278 73.624 1.00 68.16	С
ATOM	4829 NE ARG C 436	10.145 51.074 74.245 1.00 69.88	N
ATOM	4830 CZ ARG C 436	11.413 51.012 73.842 1.00 71.48	С
ATOM	4831 NH1 ARG C 436	11.753 50.206 72.835 1.00 71.96	N
ATOM	4832 NH2 ARG C 436	12.343 51.753 74.446 1.00 72.39	N
ATOM	4833 N MET C 437	9.441 45.309 74.683 1.00 65.08	N
ATOM	4834 CA MET C 437	9.124 44.123 73.919 1.00 67.98	С
ATOM	4835 C MET C 437	8.298 43.091 74.651 1.00 66.52	С
ATOM	4836 O MET C 437	7.413 42.492 74.051 1.00 67.09	0
ATOM	4837 CB MET C 437	10.394 43.416 73.489 1.00 73.78	С
ATOM	4838 CG MET C 437	11.173 44.154 72.409 1.00 80.32	С
		12.348 43.010 71.647 1.00 87.14	S
		13.497 42.566 72.961 1.00 84.82	С
ATOM	4841 N MET C 438	8.543 42.820 75.917 1.00 65.34	N
ATOM	4842 CA MET C 438	7.802 41.840 76.696 1.00 63.76	C
ATOM	4843 C MET C 438	6.488 42.370 77.246 1.00 62.74	С
ATOM	4844 O MET C 438	5.750 41.629 77.857 1.00 61.15	Ο
ATOM	4845 CB MET C 438	8.596 41.518 77.955 1.00 63.80	C
ATOM		9.993 41.010 77.625 1.00 63.23	C
ATOM		10.545 40.126 79.062 1.00 64.41	S
			С
ATOM		6.313 43.666 77.043 1.00 63.40	N
ATOM		5.120 44.358 77.478 1.00 64.21	С
ATOM		4.871 44.060 78.943 1.00 61.46	С
ATOM		3.910 43.458 79.363 1.00 60.12	0
ATOM		3.968 43.923 76.576 1.00 69.26	C
ATOM	4854 CG ASN C 439	2.734 44.729 76.957 1.00 74.42	C
ATOM		1.595 44.254 76.772 1.00 77.74	0
	4856 ND2 ASN C 439	2.935 45.937 77.509 1.00 75.66	N
	4857 N LEUC 440	5.842 44.507 79.721 1.00 59.76	N
	4858 CA LEU C 440	5.897 44.300 81.147 1.00 58.34	С
	4859 C LEU C 440	4.799 45.104 81.805 1.00 59.09	C
	4860 O LEUC 440	4.699 46.294 81.566 1.00 58.96	0
	4861 CB LEU C 440	7.262 44.697 81.689 1.00 57.06	C
	4862 CG LEU C 440	7.481 44.715 83.192 1.00 55.81	C
	4863 CD1 LEU C 440	7.505 43.319 83.760 1.00 55.18	C
	4864 CD2 LEU C 440	8.759 45.460 83.518 1.00 55.68	C
	4865 N GLN C 441	4.024 44.404 82.620 1.00 59.85	N
ATOM	4866 CA GLN C 441	2.934 45.032 83.333 1.00 60.62	С

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ATOM	4867 C GLN C 441	3.379 45.686 84.617 1.00 60.00	С
		4.368 45.251 85.170 1.00 61.05	Ο
ATOM	4869 CB GLN C 441	1.983 43.920 83.748 1.00 63.02	С
ATOM	4870 CG GLN C 441	1.311 43.221 82.594 1.00 66.39	С
ATOM	4871 CD GLN C 441	0.784 44.199 81.570 1.00 68.71	С
ATOM	4872 OE1 GLN C 441	-0.225 44.840 81.864 1.00 71.08	0
ATOM	4873 NE2 GLN C 441	1.447 44.310 80.426 1.00 69.56	N
		2.623 46.631 85.141 1.00 60.01	N
ATOM	4875 CA GLY C 442	2.979 47.285 86.401 1.00 57.82	С
ATOM	4876 C GLY C 442	2.938 46.301 87.546 1.00 56.23	С
ATOM	4877 O GLY C 442	3.773 46.384 88.432 1.00 55.56	0
ATOM	4878 N GLU C 443	2.024 45.342 87.572 1.00 56.45	N
		1.958 44.388 88.679 1.00 57.44	С
		3.253 43.564 88.662 1.00 55.03	С
		3.793 43.215 89.709 1.00 54.58	Ο
ATOM	4882 CB GLU C 443	0.788 43.422 88.734 1.00 60.73	С
		-0.627 43.920 88.621 1.00 65.19	
		-0.852 44.790 87.392 1.00 68.64	
		-0.429 44.448 86.260 1.00 69.36	
		-1.459 45.870 87.601 1.00 71.25	
		3.711 43.263 87.453 1.00 52.22	
		4.956 42.532 87.278 1.00 49.44	
		6.125 43.367 87.782 1.00 47.52	С
		6.931 42.906 88.592 1.00 47.70	O
		5.146 42.200 85.811 1.00 48.97	
		4.202 41.069 85.406 1.00 48.66	
		4.329 40.783 83.920 1.00 48.63	C
		4.480, 41.780 83.171 1.00 47.53	
		4.272 39.573 83.603 1.00 48.73	
		6.177 44.609 87.346 1.00 45.52	
ATOM	4897 CA PHE C 445	7.214 45.539 87.740 1.00 44.59 7.390 45.590 89.250 1.00 45.53	С
ATOM	4898 C PHE C 445	7.390 45.590 89.250 1.00 45.53	C
ATOM			0
		6.914 46.942 87.235 1.00 42.98	C
		7.774 48.008 87.831 1.00 42.70	C
	4902 CD1 PHE C 445		C
	4903 CD2 PHE C 445	7.246 49.026 88.586 1.00 42.91	C
	4904 CE1 PHE C 445		C
	4905 CE2 PHE C 445		C
	4906 CZ PHE C 445	9.412 49.976 88.910 1.00 44.42	C
	4907 N VAL C 446		N
		6.272 45.935 91.405 1.00 45.30	С
		6.783 44.669 92.044 1.00 46.79	C
		7.433 44.710 93.103 1.00 47.48	0
ATUM	4911 CB VAL C 446	4.837 46.404 91.699 1.00 44.57	С

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ATOM	4912	CG1 VAL C 446	4.019 45.522 92.584 1.00 43.76	C
	4913	CG2 VAL C 446	4.889 47.842 92.195 1.00 44.33	C
ATOM			6.551 43.489 91.465 1.00 47.28	N
ATOM			7.038 42.253 92.052 1.00 48.53	C
ATOM		C CYS C 447		C
ATOM			9.269 41.719 92.803 1.00 50.00	0
ATOM			6.383 41.069 91.346 1.00 50.22	C
			4.718 40.686 91.939 1.00 54.23	S
ATOM	4920	N LEU C 448	9.050 42.393 90.674 1.00 48.14	N
ATOM			10.478 42.283 90.394 1.00 45.53	C
ATOM			11.266 43.194 91.312 1.00 44.33	C
ATOM			12.270 42.813 91.897 1.00 44.64	0
ATOM	4924	CB LEU C 448	10.747 42.680 88.961 1.00 45.46	C
			10.340 41.710 87.874 1.00 46.19	C
			10.637 42.390 86.536 1.00 47.62	
			11.073 40.383 88.007 1.00 46.34	
			10.776 44.420 91.456 1.00 42.83	N
			11.442 45.371 92.343 1.00 42.54	С
			11.569 44.810 93.740 1.00 42.45	С
			12.616 44.935 94.366 1.00 42.82	0
			10.662 46.658 92.231 1.00 43.82	C
ATOM	4933	CG LYS C 449	11.518 47.902 92.420 1.00 44.96	C
ATOM	4934	CD LYS C 449	10.682 48.858 93.233 1.00 45.78	С
			9.829 49.773 92.376 1.00 45.95	С
			9.411 50.863 93.341 1.00 48.01	N
			10.585 44.140 94.330 1.00 42.30	N
ATOM	4938		10.713 43.531 95.642 1.00 41.90	С
ATOM	4939		11.654 42.334 95.600 1.00 40.58	C
ATOM	4940		12.397 42.164 96.538 1.00 41.12	0
ATOM	4941	CB SER C 450	9.389 42.962 96.170 1.00 43.19	C
			8.496 44.055 96.086 1.00 46.06	0
ATOM			11.621 41.525 94.557 1.00 39.35	N·
ATOM		CA ILE C 451	12.542 40.416 94.435 1.00 38.13	С
ATOM		C ILE C 451		C
		O ILE C 451	14.748 40.431 95.269 1.00 37.68	0
		CB ILE C 451	12.351 39.683 93.100 1.00 38.57	C
		CG1 ILE C 451	10.934 39.103 93.141 1.00 38.70	С
ATOM	4949	CG2 ILE C 451	13.459 38.678 92.856 1.00 36.53	C
ATOM		CD1 ILE C 451	10.708 38.069 92.060 1.00 40.52	C
ATOM		N ILE C 452	14.213 42.084 93.786 1.00 36.55	N
ATOM		CA ILE C 452	15.543 42.703 93.834 1.00 36.20	C
ATOM	4953	C ILE C 452	15.917 43.115 95.248 1.00 37.08	С
ATOM	4954	O ILE C 452	16.998 42.826 95.733 1.00 37.44	0
ATOM		CB ILE C 452	15.659 43.928 92.914 1.00 34.94	С
ATOM	4956	CG1 ILE C 452	15.467 43.485 91.464 1.00 35.56	С

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			_
		16.968 44.655 93.112 1.00 34.17	
		15.721 44.467 90.341 1.00 34.41	
	4959 N LEU C 453		N
		15.309 44.201 97.328 1.00 38.20	C C
	4961 C LEU C 453 4962 O LEU C 453		0
		14.114 44.954 97.944 1.00 36.92	C
		14.114 44.934 97.944 1.00 30.92	C
		15.403 46.124 99.738 1.00 33.69	C
		12.959 45.756 100.051 1.00 34.14	C
		14.922 41.886 98.094 1.00 41.70	N
		15.147 40.758 98.959 1.00 43.72	Ċ
	4969 C LEU C 454		c
ATOM	4970 O LEUC 454	•	Ō
		13.853 39.905 99.059 1.00 43.87	С
ATOM	4972 CG LEU C 454	12.778 40.568 99.923 1.00 44.26	С
ATOM	4973 CD1 LEU C 454	11.412 40.002 99.623 1.00 44.28	С
		13.149 40.345 101.376 1.00 44.75	С
_		16.464 39.630 97.230 1.00 45.86	N
		17.450 38.623 96.855 1.00 45.74	С
	4977 C ASN C 455		С
	4978 O ASN C 455		0
		17.014 37.961 95.565 1.00 44.52	C
		17.979 37.092 94.818 1.00 44.19	C
		18.469 37.593 93.781 1.00 45.37	0
		18.250 35.885 95.291 1.00 42.07 19.064 40.403 96.473 1.00 51.80	N N
		20.440 40.851 96.248 1.00 54.85	C
	4985 C SER C 456	•	c
	4986 O SER C 456		Ö
		20.435 42.295 95.736 1.00 54.12	C
		20.138 42.329 94.360 1.00 52.76	Ö
	4989 N GLY C 457	21.046 41.060 98.609 1.00 60.33	N
ATOM	4990 CA GLY C 457	21.983 40.904 99.716 1.00 63.48	С
ATOM	4991 C GLY C 457	21.824 39.630 100.506 1.00 65.50	C
ATOM	4992 O GLY C 457	22.471 39.536 101.553 1.00 65.18	0
ATOM	4993 N VAL C 458	21.007 38.692 100.047 1.00 68.21	N
	4994 CA VAL C 458	20.775 37.473 100.799 1.00 71.05	С
	4995 C VAL C 458	21.980 36.607 101.035 1.00 75.07	С
	4996 O VAL C 458	22.054 36.091 102.167 1.00 76.32	0
	4997 CB VAL C 458	19.575 36.686 100.270 1.00 69.84	C
	4998 CG1 VAL C 458	19.811 35.979 98.973 1.00 68.69	C
	4999 CG2 VAL C 458	19.138 35.706 101.359 1.00 69.73	C
	5000 N TYR C 459	22.958 36.441 100.166 1.00 79.58	N
ATOM	5001 CA TYR C 459	24.146 35.635 100.364 1.00 83.85	С

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ATOM	5002 C TYR C 459	25.224 36.366 101.129 1.00 86.14	С
ATOM	5003 O TYR C 459	26.383 35.952 101.068 1.00 87.66	Ο
ATOM	5004 CB TYR C 459	24.818 35.195 99.022 1.00 85.85	С
ATOM	5005 CG TYR C 459	23.736 34.491 98.235 1.00 88.50	С
ATOM	5006 CD1 TYR C 459	22.830 35.301 97.561 1.00 89.49	С
ATOM	5007 CD2 TYR C 459	23.534 33.123 98.179 1.00 89.54	С
ATOM	5008 CE1 TYR C 459	21.809 34.664 96.927 1.00 90.75	С
	5009 CE2 TYR C 459	22.477 32.559 97.471 1.00 90.82	С
ATOM	5010 CZ TYR C 459	21.582 33.346 96.790 1.00 91.29	C
ATOM	5011 OH TYR C 459	20.497 32.907 96.064 1.00 91.89	Ο
	5012 N THR C 460		N
ATOM	5013 CA THR C 460	25.894 38.231 102.538 1.00 91.09	С
ATOM	5014 C THR C 460	25.316 38.723 103.849 1.00 92.44	C
ATOM			О
ATOM			С
		25.703 39.507 100.413 1.00 91.84	О
		27.842 39.228 101.373 1.00 92.41	С
	5019 N PHE C 461		N
ATOM		24.018 38.287 105.816 1.00 95.54	C
ATOM	5021 C PHE C 461		C
ATOM		24.579 39.656 107.697 1.00 97.39	0
ATOM		22.859 37.323 106.179 1.00 95.11	C
ATOM	•	21.571 38.019 105.769 1.00 94.25	C
ATOM		21.517 39.404 105.732 1.00 93.75	C
ATOM		20.450 37.306 105.421 1.00 94.01	C
ATOM			C
ATOM	5028 CE2 PHE C 461	19.305 37.974 105.053 1.00 93.96	C
ATOM		19.254 39.353 105.016 1.00 93.71	С
	5030 N THR C 465		N
		24.660 32.726 112.031 1.00128.12	C
	5032 C THR C 465		C
ATOM	5033 O THR C 465		0
		25.798 31.732 112.320 1.00128.79	C
	5035 OG1 THR C 465	25.434 30.413 111.883 1.00129.06	0
	5036 CG2 THR C 465	26.164 31.714 113.795 1.00129.25	C
	5037 N LEUC 466	22.990 31.349 113.227 1.00125.02	N C
	5038 CA LEU C 466	21.700 30.665 113.350 1.00122.24	c
	5039 C LEU C 466	20.539 31.629 113.107 1.00120.10	Ö
	5040 O LEU C 466	19.510 31.214 112.557 1.00120.29 21.572 29.987 114.713 1.00122.49	C
	5041 CB LEU C 466		N
	5045 N LYS C 467	20.684 32.909 113.481 1.00116.70 19.670 33.922 113.224 1.00112.91	C
	5046 CA LYS C 467		C
	5047 C LYS C 467	19.721 34.200 111.720 1.00108.82	0
	5048 O LYS C 467	18.695 34.460 111.109 1.00108.56	C
ATOM	5049 CB LYS C 467	19.858 35.224 113.989 1.00114.52	C

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	00 7770 0 445	222/371	
		18.591 36.061 114.190 1.00115.87 18.944 37.459 114.677 1.00117.42	
		18.789 37.702 116.175 1.00117.42	
		19.336 39.016 116.623 1.00117.84	
ATOM	5054 N SER C 468	20.905 34.112 111.126 1.00103.95	N
		21.085 34.318 109.705 1.00 99.66	
		20.423 33.205 108.904 1.00 96.07	
		19.823 33.423 107.862 1.00 95.24	0
		22.564 34.322 109.314 1.00100.26	С
		23.212 35.441 109.875 1.00101.24	0
ATOM	5060 N LEUC 469	20.559 31.991 109.430 1.00 92.38	N
		19.967 30.829 108.764 1.00 89.30	C
		18.461 31.023 108.773 1.00 86.71	С
		17.766 30.720 107.816 1.00 86.34 20.473 29.539 109.400 1.00 89.33	
ATOM	5068 N GIII C 470	17.928 31.563 109.850 1.00 84.83	N
		16.495 31.823 109.972 1.00 83.61	C
		16.134 33.035 109.132 1.00 79.55	*
		15.088 33.047 108.489 1.00 78.82	O
ATOM	5072 CB GLU C 470	16.139 31.901 111.440 1.00 87.71	С
ATOM	5073 CG GLU C 470	15.292 33.077 111.873 1.00 93.24	С
		15.355 33.290 113.380 1.00 96.76	
		16.284 32.733 114.028 1.00 98.22	
		14.467 34.022 113.897 1.00 98.81	
		16.978 34.054 109.076 1.00 75.35 16.770 35.226 108.239 1.00 71.42	N C
		16.770 33.220 108.239 1.00 71.42	
ATOM	5080 O GLUC 471	16 028 35 203 105 917 1 00 70 00	Ö
ATOM	5081 CB GLU C 471	17.840 36.278 108.472 1.00 70.12	C
ATOM	5082 CG GLU C 471	17.934 36.974 109.788 1.00 68.28	С
ATOM	5083 CD GLU C 471	17.259 38.305 109.857 1.00 68.11	С
		17.694 39.296 109.273 1.00 67.82	О
		16.213 38.451 110.514 1.00 69.38	0
		17.741 33.908 106.395 1.00 68.96	N
		17.819 33.410 105.031 1.00 67.47	C
	5088 C LYS C 472 5089 O LYS C 472	16.551 32.648 104.691 1.00 65.12 16.002 32.905 103.630 1.00 64.82	C 0
	5090 CB LYS C 472	19.051 32.561 104.737 1.00 68.76	C
	5091 CG LYS C 472	20.339 33.368 104.695 1.00 70.99	Č
		21.463 32.567 104.073 1.00 73.75	Č
		22.800 32.870 104.736 1.00 76.56	Č
		23.538 34.011 104.094 1.00 78.24	N
	5095 N ASP C 473		N
		14.833 31.037 105.206 1.00 64.30	С
ATOM	5097 C ASP C 473	13.659 31.962 104.961 1.00 61.70	С

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ATOM 5187 OG1 THR C 483 9.270 33.189 92.970 1.00 49.16

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ATOM	5188	CG2 THR C 483	7.772 31.830 91.625 1.00 47.31	С
ATOM	5189	N ASP C 484	4.946 32.989 93.446 1.00 49.27	N
		CA ASP C 484		С
ATOM		C ASP C 484		С
ATOM	5192		1.876 33.608 91.893 1.00 48.21	0
ATOM	5193	CB ASP C 484	2.985 31.988 94.520 1.00 49.64	С
ATOM			3.626 30.688 94.932 1.00 51.32	С
ATOM			4.320 30.043 94.113 1.00 51.62	·O
			3.421 30.296 96.107 1.00 52.63	0
ATOM			2.869 34.912 93.360 1.00 48.09	N
ATOM			2.119 36.086 92.938 1.00 47.03	С
ATOM	5199		2.339 36.321 91.465 1.00 47.25	С
ATOM			1.385 36.554 90.749 1.00 47.41	0
ATOM			2.596 37.283 93.776 1.00 46.36	· C
			2.473 36.870 95.137 1.00 45.09	0
			1.807 38.518 93.441 1.00 45.66	С
ATOM	5204	N LEU C 486	3.584 36.243 91.012 1.00 48.22	N
ATOM.	5205	CA LEUC 486	3.918 36.449 89.612 1.00 49.46	С
ATOM	5206	C LEU C 486	3.143 35.517 88.684 1.00 50.60	С
ATOM	5207	O LEU C 486	2.431 35.935 87.777 1.00 50.21	0
ATOM	5208	CB LEU C 486	5.414 36.296 89.333 1.00 47.37	С
ATOM	5209	CG LEU C 486	6.186 37.623 89.347 1.00 46.66	С
ATOM	5210	CD1 LEU C 486	7.661 37.332 89.171 1.00 45.32	С
ATOM	5211	CD2 LEU C 486	5.628 38.632 88.358 1.00 45.13	С
ATOM			3.266 34.223 88.942 1.00 52.22	N
ATOM	5213	CA ILE C 487	2.545 33.226 88.170 1.00 53.78	С
ATOM	5214	C ILE C 487	1.043 33.494 88.230 1.00 55.38	С
ATOM	5215			0
ATOM			2.793 31.826 88.740 1.00 53.61	С
ATOM			4.243 31.431 88.572 1.00 54.10	C
ATOM	5218	CG2 ILE C 487	1.831 30.880 88.043 1.00 54.55	C
ATOM			4.670 30.922 87.218 1.00 53.75	С
ATOM			0.521 33.786 89.415 1.00 57.45	N
ATOM		CA HIS C 488	-0.879 34.089 89.597 1.00 59.38	C
		C HIS C 488	-1.279 35.176 88.603 1.00 58.99	C
		O HIS C 488	-2.211 35.056 87.824 1.00 58.98	0
		CB HIS C 488	-1.135 34.613 91.003 1.00 62.70	C
		CG HIS C 488	-2.519 35.168 91.161 1.00 65.66	C
		ND1 HIS C 488	-3.649 34.383 91.099 1.00 66.87	N
		CD2 HIS C 488	-2.948 36.439 91.363 1.00 67.13	C
		CE1 HIS C 488	-4.717 35.147 91.272 1.00 67.63	C
		NE2 HIS C 488	-4.326 36.404 91.434 1.00 67.86	N
		N LEU C 489	-0.544 36.277 88.622 1.00 58.57	N
		CA LEU C 489	-0.821 37.358 87.698 1.00 58.38	С
ATOM	5232	C LEU C 489	-0.908 36.854 86.262 1.00 58.89	С

5233 O LEUC 489	-1.829 37.140 85.507 1.00 59.10	Ο
5234 CB LEU C 489	0.330 38.360 87.856 1.00 57.52	С
		С
		С
5237 CD2 LEU C 489	-0.894 40.271 88.863 1.00 57.71	С
5238 N MET C 490	0.073 36.111 85.788 1.00 59.42	N
5239 CA MET C 490	0.185 35.601 84.450 1.00 60.66	С
5240 C MET C 490	-0.958 34.696 84.016 1.00 62.10	С
5241 O MET C 490	-1.461 34.765 82.892 1.00 62.62	Ο
		С
		С
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		N
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5269 N LEUC 495	-2.156 33.035 80.240 1.00 69.12	N
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		C
		O C
5281 CB THR C 496	0.131 28.249 //.679 1.00 69.65	C
	5234 CB LEU C 489 5235 CG LEU C 489 5236 CD1 LEU C 489 5237 CD2 LEU C 489 5238 N MET C 490 5239 CA MET C 490 5240 C MET C 490 5241 O MET C 490 5242 CB MET C 490 5243 CG MET C 490 5244 SD MET C 490 5245 CE MET C 490 5246 N ALA C 491 5247 CA ALA C 491 5248 C ALA C 491 5249 O ALA C 491 5250 CB ALA C 491 5251 N LYS C 492 5252 CA LYS C 492 5253 C LYS C 492 5254 O LYS C 492 5255 CB LYS C 492 5255 CB LYS C 492 5256 N ALA C 493 5261 CA ALA C 493 5262 C ALA C 493 5263 O ALA C 493 5264 CB ALA C 493 5265 N GLY C 494 5266 CA GLY C 494 5266 CA GLY C 494 5267 C GLY C 494 5268 O GLY C 494 5269 N LEU C 495 5270 CA LEU C 495 5271 C LEU C 495 5271 C LEU C 495 5273 CB LEU C 495 5274 CG LEU C 495 5275 CD1 LEU C 495 5276 CD2 LEU C 495 5277 N THR C 496 5278 CA THR C 496 5279 C THR C 496	5234 CB LEU C 489 5235 CG LEU C 489 5236 CD1 LEU C 489 5237 CD2 LEU C 489 5238 N MET C 490 5239 CA MET C 490 5241 O MET C 490 5241 O MET C 490 5242 CB MET C 490 5244 SD MET C 490 5245 CE MET C 490 5246 N ALA C 491 5246 N ALA C 491 5247 CA ALA C 491 5248 C ALA C 491 5252 CB ALA C 491 5253 C LYS C 492 5253 C LYS C 492 5253 C LYS C 492 5254 O LYS C 492 5255 CB LYS C 492 5256 O ALA C 493 5260 N ALA C 493 5261 CA ALA C 493 5262 C ALA C 493 5263 O ALA C 493 5264 CB ALA C 493 5265 N GLY C 494 5266 CA GLY C 494 5266 CA GLY C 494 5267 C GLY C 494 5268 O GLY C 494 5268 O GLY C 494 5269 N LEU C 495 5277 CB LEU C 495 5277 CT THR C 496 5278 CA THR C 496 5278 CA THR C 496 5278 CA THR C 496 5279 C THR C 496 5277 C THR C 496

wo	98/568	312		PCT
			227/371	
ATOM	5282	OG1 THR C 496	-0.649 28.629 76.549 1.00 70.83	0
ATOM		CG2 THR C 496	0.241 26.748 77.746 1.00 71.54	С
ATOM		N LEU C 497	0.243 27.387 80.603 1.00 70.09	N
ATOM		CA LEU C 497	1.104 26.974 81.695 1.00 70.17	С
ATOM		C LEU C 497	2.554 27.015 81.241 1.00 70.38	C
ATOM		O LEU C 497	3.468 27.257 82.022 1.00 70.44	0
ATOM		CB LEU C 497	0.734 25.569 82.077 1.00 71.33	C
ATOM		CG LEU C 497	0.560 25.185 83.533 1.00 72.65	C C
ATOM		CD1 LEU C 497	1.474 23.971 83.684 1.00 73.62 0.900 26.296 84.517 1.00 73.68	C
ATOM		CD2 LEU C 497 N GLN C 498	2.790 26.779 79.954 1.00 71.07	N
ATOM ATOM		CA GLN C 498	4.125 26.835 79.385 1.00 71.07	Ċ
ATOM		C GLN C 498	4.522 28.281 79.136 1.00 69.80	c
		O GLN C 498	5.688 28.601 79.316 1.00 70.90	Ö
		CB GLN C 498	4.285 26.031 78.110 1.00 72.84	C
ATOM		CG GLN C 498	5.423 26.529 77.246 1.00 76.47	C
ATOM		CD GLN C 498	5.789 25.674 76.064 1.00 78.75	С
ATOM		OE1 GLN C 498	6.954 25.383 75.787 1.00 79.93	0
ATOM	5300	NE2 GLN C 498	4.808 25.224 75.292 1.00 80.37	N
ATOM		N GLN C 499	3.637 29.190 78.769 1.00 68.09	N
ATOM		CA GLN C 499	4.045 30.579 78.566 1.00 66.52	С
		C GLN C 499	4.335 31.222 79.916 1.00 65.14	C
		O GLN C 499	5.128 32.156 80.000 1.00 65.15	0
ATOM		CB GLN C 499	2.954 31.403 77.908 1.00 67.39	C C
ATOM		CG GLN C 499 CD GLN C 499	2.187 30.566 76.902 1.00 68.26 1.351 31.474 76.031 1.00 69.04	C
ATOM ATOM		OE1 GLN C 499	0.360 32.015 76.504 1.00 69.68	O
ATOM		NE2 GLN C 499	1.831 31.578 74.804 1.00 69.76	N
ATOM		N GLN C 500	3.651 30.693 80.931 1.00 62.78	N
		CA GLN C 500	3.837 31.173 82.288 1.00 60.68	С
ATOM		C GLN C 500	5.280 30.888 82.701 1.00 58.45	С
		O GLN C 500	6.001 31.837 83.021 1.00 58.31	0
ATOM	5314	CB GLN C 500	2.885 30.508 83.254 1.00 61.20	С
		CG GLN C 500	1.505 31.146 83.337 1.00 62.27	C
		CD GLN C 500	0.578 30.080 83.904 1.00 63.04	C
		OE1 GLN C 500	0.821 29.501 84.963 1.00 63.59	0
		NE2 GLN C 500	-0.480 29.815 83.175 1.00 63.65	N
		N HIS C 501	5.709 29.635 82.623 1.00 55.31	N C
			7.082 29.352 83.006 1.00 53.62 8.090 30.065 82.126 1.00 53.32	c
		C HIS C 501 O HIS C 501	9.177 30.418 82.628 1.00 54.43	o
		CB HIS C 501	7.384 27.886 83.164 1.00 53.44	C
			7.433 26.979 81.994 0.50 52.73	C
			6.349 27.013 83.805 0.50 53.70	Č
		ND1AHIS C 501	6.855 25.722 82.044 0.50 52.67	N

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ATOM	5372	CG AGLN C 506	10.997 35.027 79.008 0.30 49.22	C
ATOM	5373	CG BGLN C 506	11.982 35.439 78.402 0.50 47.09	С
ATOM	5374	CD AGLN C 506	10.287 35.261 77.712 0.50 50.52	С
ATOM	5375	CD BGLN C 506	13.443 35.396 78.009 0.50 47.98	С
ATOM	5376	OE1AGLN C 506	9,576 36,260 77,534 0.50 51.64	Ο .
ATOM	5377	OE1BGLN C 506	14.172 36.371 78.271 0.50 49.11	0
ATOM	5378	NE2AGLN C 506	10.462 34.314 76.787 0.50 50.82	N
ATOM	5379	NE2BGLN C 506	13.898 34.308 77.392 0.50 46.84	N
			11.595 37.106 82.794 1.00 47.02	
			11.637 38.214 83.728 1.00 46.79	
ATOM	5382	C LEUC 507	12.799 38.120 84.695 1.00 46.70	С
ATOM	5383	O LEU C 507	13.560 39.089 84.808 1.00 48.95	0
ATOM	5384	CB LEU C 507	10.352 38.324 84.531 1.00 48.26	С
ATOM	5385	CG LEU C 507	10.352 38.324 84.531 1.00 48.26 9.117 38.715 83.712 1.00 49.58	С
ATOM	5386	CD1 LEU C 507	7.913 38.843 84.649 1.00 50.04	C
ATOM	5387	CD2 LEU C 507	9.362 40.006 82.960 1.00 49.77	С
			12.972 37.000 85.367 1.00 45.26	
ATOM	5389	CA LEU C 508	14.095 36.831 86.281 1.00 43.54	С
ATOM	5390	C LEUC 508	15.415 36.889 85.546 1.00 42.79	С
ATOM	5391	O LEUC 508	16.349 37.442 86.161 1.00 44.62	O
ATOM	5392	CB LEU C 508	13.903 35.535 87.070 1.00 43.30	C
ATOM	5393	CG LEU C 508	12.574 35.493 87.827 1.00 42.75	C
ATOM	5394	CD1 LEU C 508	12.432 34.160 88.525 1.00 45.27	C
ATOM	5395	CD2 LEU C 508	12.528 36.588 88.857 1.00 43.71	C
ATOM	5396	N LEUC 509	15.593 36.440 84.302 1.00 40.58	N
ATOM	5397	CA LEU C 509	16.930 36.594 83.716 1.00 40.98	С
ATOM	5398	C LEU C 509	17.371 38.056 83.559 1.00 41.80	C
ATOM	5399	O LEUC 509	18.571 38.373 83.557 1.00 40.85	0
ATOM	5400	CB LEU C 509	17.133 35.825 82.417 1.00 39.19	C
ATOM	5401	CG LEU C 509	17.199 34.314 82.518 1.00 38.43 17.193 33.742 81.124 1.00 38.49	С
ATOM	5402	CDI LEU C 509	17.193 33.742 81.124 1.00 38.49	C C
			18.408 33.853 83.302 1.00 38.49	N · · · · ·
			16.437 39.005 83.446 1.00 42.22	C
			16.736 40.420 83.312 1.00 41.83	c
		C ILEC 510	17.415 40.875 84.591 1.00 41.01 18.297 41.731 84.568 1.00 41.48	0
		O ILEC 510	15.521 41.794 82.999 1.00 41.89	C
		CB ILE C 510 CG1 ILE C 510	15.237 41.294 82.999 1.00 41.89	C
		CG2 ILE C 510	15.738 42.756 83.300 1.00 41.62	č
		CD1 ILE C 510	13.765 41.061 81.156 1.00 47.45	Č
		N LEUC 511	17.034 40.302 85.721 1.00 40.64	N
			17.645 40.700 86.982 1.00 41.72	C
		C LEU C 511	19.161 40.571 86.924 1.00 42.18	c
		O LEUC 511	19.883 41.400 87.487 1.00 43.39	Ö
		CB LEU C 511	17.051 39.931 88.151 1.00 41.42	C
AT OW	2410	CD DEC COIL	1,.001 07.701 00.101 1.00 .1.10	-

wo	98/56812	230/371	PCT/GB98/01708
ATOM	5417 CG LEU C 511	15.549 40.136 88.361 1.00 41.22	С
ATOM	5418 CD1 LEU C 511	15.186 39.555 89.731 1.00 41.54 15.150 41.585 88.240 1.00 39.85	С
ATOM	5419 CD2 LEU C 511	15.150 41.585 88.240 1.00 39.85	С
ATOM	5420 N SER C 512	19.719 39.597 86.239 1.00 41.63	N
ATOM	5421 CA SER C 512	21.143 39.455 86.122 1.00 41.44	С
ATOM	5422 C SER C 512	21.758 40.706 85.513 1.00 41.95	С
		22.722 41.284 86.035 1.00 42.95	0
ATOM	5424 CB SER C 512	21.414 38.338 85.114 1.00 43.11	С
ATOM	5425 OG SER C 512	22.472 37.616 85.722 1.00 47.13	0
ATOM	5426 N HIS C 513	21.211 41.137 84.368 1.00 40.29	N
ATOM	5427 CA HIS C 513	21.684 42.330 83.681 1.00 37.65	С
ATOM	5428 C HIS C 513	21.571 43.508 84.623 1.00 38.21	С
ATOM	5429 O HIS C 513	22.529 44.283 84.760 1.00 38.29	
		20.913 42.523 82.391 1.00 37.61	С
ATOM	5431 CG AHIS C 513	21.265 41.340 81.520 0.50 38.24	C
ATOM	5432 CG BHIS C 513	21.461 43.588 81.495 0.50 39.47	C
ATOM	5433 ND1AHIS C 513	20.348 40.481 80.972 0.50 38.41	N
ATOM	5434 ND1BHIS C 513	20.716 44.626 80.974 0.50 39.63	N
		22.479 40.878 81.129 0.50 38.68	
ATOM	5436 CD2BHIS C 513	22.721 43.759 80.999 0.50 40.24	C
ATOM	5437 CE1AHIS C 513	20.978 39.547 80.280 0.50 38.17	C
ATOM	5438 CE1BHIS C 513	21.484 45.382 80.212 0.50 40.30	C
ATOM	5439 NE2AHIS C 513	22.272 39.767 80.352 0.50 38.14	N
ATOM	5440 NEZBHIS C 513	22.716 44.877 80.208 0.30 40.60	14
ATOM	5441 N ILE C 514	20.451 43.655 85.332 1.00 37.46	N
ATOM	5442 CA ILEC 514	20.347 44.761 86.284 1.00 37.60	C
ATOM	5443 C ILE C 514	21.468 44.626 87.289 1.00 37.99	C
		22.180 45.604 87.576 1.00 38.56	
ATOM	5445 CB ILE C 514	18.949 44.788 86.900 1.00 38.83	
ATOM	5446 CGI ILE C 514	17.942 45.260 85.827 1.00 39.26 18.836 45.675 88.137 1.00 38.87	C
ATOM	5447, CG2 ILE C 514	16.544 44.724 86.101 1.00 37.40	C
	5449 N ARG C 515	21.778 43.442 87.821 1.00 38.49	N
	5450 CA ARG C 515	22.918 43.325 88.749 1.00 38.93	C
	5451 C ARG C 515	24.180 43.899 88.089 1.00 39.23	c .
	5452 O ARG C 515	24.857 44.762 88.618 1.00 37.78	Ö
	5453 CB ARG C 515	23.205 41.877 89.137 1.00 38.60	Č
	5454 CG ARG C 515	24.107 41.682 90.328 1.00 39.98	Č
	5455 CD ARG C 515	23.553 42.402 91.524 1.00 42.75	Č
	5456 NE ARG C 515	23.858 41.831 92.818 1.00 45.59	N
	5457 CZ ARG C 515		Ċ
	5458 NH1 ARG C 515		N
	5459 NH2 ARG C 515		N
	5460 N HIS C 516	24.442 43.367 86.880 1.00 38.97	N
	5461 CA HIS C 516	25.559 43.743 86.079 1.00 37.57	C

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ATOM	5462 C HIS C 516	25.669 45.231 85.924 1.00 37.44	С
ATOM	5463 O HIS C 516	26.724 45.772 86.137 1.00 36.85	0
		25.484 43.088 84.675 1.00 39.10	С
ATOM	5465 CG HIS C 516	5 26.800 43.430 83.987 1.00 39.84	С
ATOM	5466 ND1 HIS C 51	6 28.000 42.830 84.270 1.00 38.68	N
ATOM	5467 CD2 HIS C 51	6 27.067 44.373 83.053 1.00 39.95	С
ATOM	5468 CE1 HIS C 510	6 28.926 43.374 83.556 1.00 38.48	С
ATOM	5469 NE2 HIS C 51	6 28.402 44.310 82.802 1.00 39.09	N
ATOM	5470 N MET C 51	7 24.624 45.905 85.507 1.00 40.05	N
ATOM	5471 CA MET C 51	24.581 47.349 85.315 1.00 41.49	С
ATOM	5472 C MET C 517	7 24.887 48.141 86.576 1.00 41.19	С
ATOM	5473 O MET C 51	7 25.656 49.088 86.572 1.00 40.45	0
ATOM	5474 CB MET C 51	23.133 47.749 84.952 1.00 42.86	C
ATOM	5475 CG MET C 51	17 23.062 48.179 83.500 1.00 44.59 7 21.375 48.400 82.948 1.00 45.13	С
ATOM	5476 SD MET C 51	21.375 48.400 82.948 1.00 45.13	S
		7 20.821 46.716 83.021 1.00 47.50	
ATOM	5478 N SER C 518	24.242 47.713 87.662 1.00 41.17	N
ATOM	5479 CA SER C 51	8 24.431 48.350 88.959 1.00 42.10	C .
		25.900 48.293 89.378 1.00 41.62	
		26.435 49.226 89.972 1.00 40.04	0
ATOM	5482 CB SER C 51	8 23.515 47.681 89.976 1.00 43.27	С
ATOM	5483 OG SER C 51	8 24.029 47.552 91.289 1.00 44.28	0
		26.559 47.178 89.096 1.00 42.60	
		9 27.949 46.967 89.451 1.00 44.06	
		28.745 47.991 88.681 1.00 45.41	C O
ATOM	5487 O ASN C 519	29.549 48.667 89.315 1.00 47.80	
ATOM	5488 CB ASN C 51	9 28.448 45.555 89.206 1.00 45.80 9 28.018 44.580 90.279 1.00 47.88	C
ATOM	5489 CG ASN C 51	19 27.926 45.010 91.435 1.00 50.31	
ATOM	5490 OD1 ASN C 5	19 27.732 43.312 90.024 1.00 48.12	
ATOM	5491 ND2 ASIN C 3	28.523 48.167 87.396 1.00 45.89	N
		0 29.236 49.176 86.629 1.00 46.46	
	5494 C LYS C 520		C
	5495 O LYS C 520		Ö
	5496 CB LYS C 52		C
	5497 CG LYS C 52		C
	5498 CD LYS C 52		C
	5499 CE LYS C 52		C
	5500 NZ LYS C 52		N
	5501 N GLY C 52	·	N
	5502 CA GLY C 52		С
	5503 C GLY C 52		С
	5504 O GLY C 52		О
	5505 N MET C 52		N
	5506 CA MET C 52		С

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		232/371	
		30.253 52.370 90.993 1.00 48.58	C O
	5508 O MET C 522	30.785 53.372 91.449 1.00 49.59 29.054 51.248 92.623 1.00 46.05	
		28.178 50.220 93.195 1.00 47.14	c
		26.835 50.822 94.200 1.00 48.30	
ATOM	5512 CE MET C 522	27.488 52.344 94.834 1.00 47.03	Č
		30.839 51.485 90.186 1.00 50.74	
		32.219 51.708 89.771 1.00 50.96	
		32.345 53.103 89.211 1.00 47.76	С
ATOM	5516 O GLU C 523	33.253 53.809 89.603 1.00 47.73	·O
		32.667 50.627 88.824 1.00 56.55	
ATOM	5518 CG GLU C 523	33.327 49.441 89.503 1.00 64.56	С
ATOM	5519 CD GLU C 523	34.430 49.763 90.500 1.00 69.18	C
ATOM	5520 OE1 GLU C 523	34.979 50.901 90.485 1.00 71.53	
		34.775 48.861 91.321 1.00 71.46	0
		31.443 53.541 88.377 1.00 45.46	N
		31.422 54.860 87.801 1.00 45.10	C
ATOM	5524 C FIIS C 524	31.139 55.989 88.775 1.00 45.54	C
		31.760 57.047 88.813 1.00 43.84 30.302 54.867 86.714 1.00 44.35	C
		30.172 56.201 86.043 1.00 43.95	
ATOM	5528 ND1 HIS C 524	29 392 57 207 86 582 1.00 44.66	N
ATOM	5529 CD2 HIS C 524	29.392 57.207 86.582 1.00 44.66 30.702 56.715 84.921 1.00 43.61	C
ATOM	5530 CE1 HIS C 524	29.451 58.282 85.815 1.00 44.69	С
		30.246 58.006 84.791 1.00 44.31	
ATOM	5532 N LEUC 525	30.129 55.837 89.635 1.00 47.24	
		29.737 56.875 90.572 1.00 49.14	С
		30.940 57.158 91.461 1.00 52.11	C
ATOM	5535 O LEU C 525	31.220 58.281 91.867 1.00 52.94	0
		28.524 56.521 91.430 1.00 47.83	C
	5537 CG LEU C 525	28.177 57.531 92.529 1.00 46.65	C
	5538 CD1 LEU C 525 5539 CD2 LEU C 525	27.759 58.851 91.904 1.00 46.66 27.043 57.027 93.393 1.00 46.47	C C
	5540 N TYR C 526	31.622 56.068 91.767 1.00 54.77	N
	5541 CA TYR C 526	32.813 56.096 92.574 1.00 57.68	C
	5542 C TYR C 526	33.902 56.853 91.852 1.00 58.29	c
	5543 O TYR C 526	34.445 57.709 92.533 1.00 59.72	Ō
	5544 CB TYR C 526	33.217 54.646 92.801 1.00 61.45	С
ATOM	5545 CG TYR C 526	34.415 54.632 93.718 1.00 64.71	C
	5546 CD1 TYR C 526	34.244 54.801 95.071 1.00 66.72	С
	5547 CD2 TYR C 526	35.679 54.461 93.207 1.00 66.45	C
	5548 CE1 TYR C 526		C
	5549 CE2 TYR C 526	36.771 54.443 94.040 1.00 68.71	C
ATOM		36.573 54.604 95.385 1.00 70.11	С
ATOM	5551 OH TYR C 526	37.667 54.593 96.230 1.00 74.04	0

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		234/371	
		33.576 65.532 91.235 1.00 85.41	
		32.575 66.043 90.328 1.00 83.84	C
		31.192 65.917 90.966 1.00 84.07	C
		30.192 66.581 90.690 1.00 85 .18 32.587 65.178 89.053 1.00 83 .29	O C
ATOM	5604 CG1 VAL C 533	31.687 65.744 87.979 1.00 83.42	C
		33.980 64.923 88.521 1.00 82.88	C
		31.094 64.963 91.882 1.00 83.18	N
		29.895 64.631 92.612 1.00 82.16	
		29.866 65.401 93.925 1.00 81.49	C
		30.817 65.427 94.693 1.00 80.19	O
ATOM	5610 CB VAL C 534	29.905 63.124 92.979 1.00 83.14	С
ATOM	5611 CG1 VAL C 534	28.769 62.657 93.896 1.00 82.66	С
		29.879 62.310 91.680 1.00 83.87	С
	5613 N PRO C 535		N
		28.413 66.702 95.382 1.00 82.22	С
	5615 C PRO C 535		C
		28.315 64.471 96.489 1.00 82.55	0
		27.037 67.375 95.227 1.00 81.89	C
		26.639 67.049 93.824 1.00 81.50 27.549 65.969 93.280 1.00 81.99	
	5620 N LEU C 536		N
	5621 CA LEU C 536	28.458 65.656 99.010 1.00 85.26	C
	5622 C LEU C 536		c
	5623 O LEUC 536		O
	5628 N TYR C 537		N
		24.946 64.232 99.320 1.00 78.85	С
		25.325 63.093 100.266 1.00 76.77	С
ATOM	5631 O TYR C 537	26.030 62.171 99.878 1.00 75.21	0
ATOM	5632 CB TYR C 537	23.950 63.823 98.270 1.00 79.38	С
	5633 CG TYR C 537	23.674 64.920 97.266 1.00 80.32	C
	5634 CD1 TYR C 537	23.077 66.101 97.666 1.00 80.91	C
	5635 CD2 TYR C 537		C
	5636 CE1 TYR C 537	22.810 67.113 96.765 1.00 81.66	C
	5637 CE2 TYR C 537 5638 CZ TYR C 537	23.725 65.799 95.029 1.00 81.20 23.135 66.962 95.437 1.00 81.56	C C
	5639 OH TYR C 537	22.870 67.969 94.533 1.00 82.05	0
	5640 N ASP C 538	24.878 63.218 101.503 1.00 75.21	N
	5641 CA ASP C 538	25,123 62,267 102,558 1.00 72.00	C
	5642 C ASP C 538	24.514 60.891 102.464 1.00 66.75	c
	5643 O ASP C 538	25.237 59.938 102.741 1.00 65.15	Ö
	5644 CB ASP C 538	24.546 62.905 103.842 1.00 77.25	C
	5645 CG ASP C 538	25.685 63.756 104.406 1.00 82.29	С
ATOM	5646 OD1 ASP C 538	26.854 63.294 104.279 1.00 84.32	0
ATOM	5647 OD2 ASP C 538	25.382 64.854 104.952 1.00 85.06	0

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	5648 N LEU C 539	23.237 60.800 102.109 1.00 61.50	N
	5649 CA LEU C 539	22.614 59.463 102.040 1.00 57.70	C
	5650 C LEU C 539	23.202 58.654 100.888 1.00 56.49	C
	5651 O LEU C 539	23.415 57.430 101.038 1.00 56.40	0
	5652 CB LEU C 539	21.094 59.590 102.037 1.00 54.92	C
		20.181 58.390 102.109 1.00 52.57	C
		20.588 57.443 103.233 1.00 52.85	C
ATOM		18.728 58.797 102.254 1.00 51.12	C
ATOM		23.470 59.331 99.765 1.00 53.82	N
	5657 CA LEU C 540	24.051 58.684 98.609 1.00 51.49	С
	5658 C LEU C 540	25.475 58.264 98.937 1.00 51.94	C
ATOM		25.864 57.132 98.631 1.00 51.62	0
ATOM	5660 CB LEU C 540	24.025 59.601 97.402 1.00 50.54	C
		24.540 59.050 96.072 1.00 49.41	C
		23.497 58.167 95.415 1.00 49.15	C
	5663 CD2 LEU C 540	24.920 60.162 95.125 1.00 49.22	C
	5664 N LEU C 541	26.295 59.070 99.606 1.00 52.86	N
	5665 CA LEU C 541	27.647 58.590 99.900 1.00 54.81	C
	5666 C LEU C 541	27.583 57.402 100.833 1.00 54.48	С
ATOM		28.422 56.498 100.786 1.00 55.31	0
ATOM		28.610 59.697 100.352 1.00 57.53	C
ATOM	5669 CG LEU C 541	28.653 60.816 99.296 1.00 61.05	C
		29.463 62.019 99.757 1.00 62.25	C
	5671 CD2 LEU C 541	29.114 60.322 97.917 1.00 61.64	C
ATOM		26.595 57.350 101.704 1.00 53.99	N
ATOM		26.418 56.251 102.640 1.00 52.85	C
	5674 C GLU C 542	26.178 54.974 101.861 1.00 51.65	C
	5675 O GLU C 542	26.961 54.046 102.029 1.00 51.91	0
ATOM		25.230 56.537 103.529 1.00 54.48	C C
		25.010 55.532 104.650 1.00 56.13	C
	5678 CD GLUC 542	23.909 56.070 105.555 1.00 57.89	
	5679 OE1 GLU C 542	23.891 57.334 105.706 1.00 59.80	0
	5680 OE2 GLU C 542	23.135 55.235 106.045 1.00 57.42	O N
	5681 N MET C 543	25.172 54.915 101.007 1.00 50.30 24.941 53.723 100.201 1.00 49.51	C
	5682 CA MET C 543	26.134 53.388 99.327 1.00 49.84	C
	5683 C MET C 543	26.476 52.234 99.063 1.00 49.91	O
	5684 O MET C 543	23.707 54.018 99.348 1.00 50.39	C
	5685 CB MET C 543	22.554 54.449 100.251 1.00 51.60	C
	5686 CG MET C 543	21.911 53.008 101.129 1.00 53.05	S
	5687 SD MET C 543	22.145 53.467 102.831 1.00 52.49	C
	5688 CE MET C 543 5689 N LEU C 544	26.855 54.372 98.805 1.00 50.40	N
		28.028 54.108 97.979 1.00 51.36	C
	5690 CA LEU C 544 5691 C LEU C 544	29,130 53,494 98.826 1.00 52.36	c
		29.752 52.546 98.374 1.00 51.79	Ö
ATOM	3032 U LEU C 344	45.134 34.340 30.314 1.00 31.19	•

19.869 58.501 89.282 1.00 35.71

18.524 58.409 89.623 1.00 37.42

17.822 57.308 89.220 1.00 38.32

16.483 57.175 89.546 1.00 38.91

18.405 56.280 88.463 1.00 38.39

19.774 56.391 88.128 1.00 36.82

C

C

C

O C

TER 5731

ARG C 548

HETATM 5732 C1 EST C 600

HETATM 5733 C2 EST C 600

HETATM 5734 C3 EST C 600

HETATM 5735 O3 EST C 600

HETATM 5736 C4 EST C 600

HETATM 5737 C5 EST C 600

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TTT ATT 4 5729 C6 FST C 600	237/371 20.294 55.421 87.091 1.00 37.10	С
HETATM 5738 C6 EST C 600 HETATM 5739 C7 EST C 600	21.704 55.728 86.604 1.00 36.50	Č
HETATM 5740 C8 EST C 600	22.535 56.278 87.762 1.00 36.05	Č
HETATM 5741 C9 EST C 600		
HETATM 5742 C10 EST C 600	20.489 57.499 88.548 1.00 35.28	
HETATM 5743 C11 EST C 600		С
HETATM 5744 C12 EST C 600	24.163 58.593 88.768 1.00 35.50	
HETATM 5745 C13 EST C 600	24.772 57.250 88.396 1.00 35.67	
HETATM 5746 C14 EST C 600		
HETATM 5747 C15 EST C 600	24.852 55.358 87.058 1.00 35.36	C
HETATM 5748 C16 EST C 600	26.207 56.101 86.772 1.00 36.43	C
HETATM 5749 C17 EST C 600	26.129 57.338 87.694 1.00 36.25	C
HETATM 5750 O17 EST C 600	27.295 57.444 88.500 1.00 35.57	0
HETATM 5751 C18 EST C 600	24.895 56.358 89.623 1.00 35.57	C
ATOM 5752 N SER D 305	17.263 25.806 62.987 1.00 89.17	N
ATOM 5753 CA SER D 305	18.225 25.610 64.101 1.00 88.43	C
ATOM 5754 C SER D 305	17.959 24.319 64.864 1.00 87.99	C
ATOM 5/55 O SER D 305	16.871 24.093 65.388 1.00 87.53 18.202 26.835 65.025 1.00 88.28	C
ATOM 5757 OG SER D 305	19.076 26.687 66.122 1.00 88.48	0
ATOM 5757 N I FILD 306	18.986 23.473 64.970 1.00 87.77	N
ATOM 5750 CA LEUD 306	18.892 22.224 65.722 1.00 87.21	C
ATOM 5760 C LEU D 306		C
ATOM 5761 O LEU D 306	17.265 22.095 67.508 1.00 85.96	0
ATOM 5762 CB LEU D 306	20.260 21.563 65.896 1.00 87.76	С
	18.916 23.530 67.764 1.00 83.98	N
ATOM 5767 CA ALA D 307	18.454 24.030 69.037 1.00 82.92	С
ATOM 5768 C ALA D 307	16.936 , 23.984 69.095 1.00 81.76	С
ATOM 5769 O ALA D 307	16.381 23.264 69.911 1.00 81.64	0
	18.859 25.491 69.224 1.00 83.73	C
ATOM 5771 N LEU D 308	16.268 24.720 68.224 1.00 81.06	N
	14.821 24.770 68.211 1.00 80.81	С
	14.111 23.495 67.849 1.00 81.21	C
ATOM 5774 O LEU D 308	12.876 23.519 67.861 1.00 83.27	0
ATOM 5775 CB LEU D 308	14.399 25.920 67.280 1.00 80.70 14.927 27.298 67.651 1.00 80.94	C C
ATOM 5776 CG LEU D 308	14.130 28.397 66.971 1.00 80.94	C
ATOM 5777 CD1 LEU D 308 ATOM 5778 CD2 LEU D 308	14.130 28.397 66.971 1.00 81.19	Č
ATOM 5778 CD2 LEO D 308 ATOM 5779 N SER D 309	14.715 22.378 67.525 1.00 80.53	N
ATOM 5779 N SER D 309 ATOM 5780 CA SER D 309	14.075 21.138 67.169 1.00 79.50	C
ATOM 5780 CA SER D 309	14.253 20.044 68.198 1.00 78.69	c
ATOM 5782 O SER D 309	13.378 19.186 68.319 1.00 79.89	0
ATOM 5783 CB SER D 309	14.740 20.609 65.891 1.00 80.73	С
ATOM 5784 OG SER D 309	14.751 21.696 64.969 1.00 83.38	0
ATOM 5785 N LEU D 310	15.383 20.027 68.902 1.00 76.78	N

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ATOM	5786 CA LEUD 310	15.586 18.976 69.894 1.00 74.02	С
ATOM	5787 C LEU D 310	14.459 19.034 70.927 1.00 72.78	С
ATOM	5788 O LEUD 310	13.795 20.037 71.154 1.00 72.43	O
		16.950 19.048 70.540 1.00 73.54	
ATOM	5790 CG LEU D 310	18.073 19.617 69.677 1.00 72.90	С
ATOM	5791 CD1 LEU D 310	18.593 20.870 70.346 1.00 73 .00 19.183 18.589 69.545 1.00 73 .78	С
ATOM	5792 CD2 LEU D 310	19.183 18.589 69.545 1.00 73.78	С
		14.248 17.880 71.528 1.00 71.14	
ATOM	5705 C TUD D 211	13.223 17.687 72.536 1.00 69.71	
ATOM	5796 O THR D 311	13.896 17.914 73.860 1.00 69.14 15.114 17.705 73.880 1.00 69.46	C O
		12.696 16.259 72.386 1.00 70.04	
ATOM	5798 OG1 THR D 311	13.681 15.274 72.691 1.00.69.74	0
ATOM	5799 CG2 THR D 311	12.246 16.024 70.952 1.00 69.87	Č
ATOM	5800 N ALA D 312	12.246 16.024 70.952 1.00 69.87 13.215 18.263 74.934 1.00 68.71	N
ATOM	5801 CA ALA D 312	13.912 18.480 76.198 1.00 68.63	С
ATOM	5802 C ALA D 312	14.925 17.380 76.447 1.00 68.98	С
ATOM	5803 O ALA D 312	16.044 17.697 76.851 1.00 69.24 12.983 18.641 77.366 1.00 68.89	0
ATOM	5804 CB ALA D 312	12.983 18.641 77.366 1.00 68.89	C
		14.592 16.129 76.206 1.00 70.40	
ATOM	5807 C ASP D 313	15.559 15.061 76.417 1.00 72.08	C C
ATOM	5808 O ASP D 313	16.794 15.157 75.562 1.00 69.74 17.855 14.913 76.108 1.00 68.84	0
ATOM	5809 CB ASP D 313	14.902 13.680 76.231 1.00 76.64	
ATOM	5810 CG ASP D 313	14.055 13.442 77.472 1.00 80.32	С
ATOM	5811 OD1 ASP D 313	14.677 13.473 78.554 1.00 82.36	0
ATOM	5812 OD2 ASP D 313	14.677 13.473 78.554 1.00 82.36 12.822 13.267 77.370 1.00 82.59	0
ATOM	5813 N GLN D 314	16.722 15.478 74.298 1.00 69.16	N
ATOM	5814 CA GLN D 314	17.892 15.578 73.433 1.00 69.14	С
		18.762 16.748 73.860 1.00 67.43	
	5816 O GLN D 314 5817 CB GLN D 314	19.983 16.632 73.906 1.00 67.85	0
	5818 CG GLN D 314	17.494 15.775 71.972 1.00 71.65 16.256 14.951 71.631 1.00 74.11	C C
	5819 CD GLN D 314	15.887 15.055 70.179 1.00 76.25	C
	5820 OE1 GLN D 314	14.964 15.747 69.756 1.00 77.94	Ö
	5821 NE2 GLN D 314	16.681 14.318 69.406 1.00 77.91	N
ATOM	5822 N MET D 315	18.104 17.860 74.181 1.00 64.64	N
	5823 CA MET D 315	18.765 19.058 74.684 1.00 60.92	С
	5824 C MET D 315	19.646 18.678 75.867 1.00 58.71	С
	5825 O MET D 315	20.853 18.867 75.830 1.00 57.58	0
	5826 CB MET D 315	17.704 20.050 75.130 1.00 60.65	C
	5827 CG MET D 315 5828 SD MET D 315	18.233 21.397 75.579 1.00 61.16	C
	5829 CE MET D 315	18.673 22.508 74.236 1.00 60.09 20.398 22.700 74.561 1.00 60.98	S C
ATOM		19.068 18.104 76.912 1.00 57.26	N
	110011 111100010	17.000 10.104 /0.712 1,00 37.20	44

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4 TO 8 4	5021 CA VAI D 216	19.812 17.687 78.077 1.00 57.08	С
ATOM	5832 C VAL D 316	21 023 16 839 77 740 1 00 58 01	Č
ATOM	5833 O VAL D 316	21.023 16.839 77.740 1.00 58.01 22.096 17.031 78.310 1.00 58.94	Ö
ATOM	5834 CB VALD 316	18.988 16.858 79.081 1.00 56.33	C
ATOM	5835 CG1 VAL D 316	19.824 16.374 80.254 1.00 55.69	
ATOM	5836 CG2 VAL D 316	17.844 17.705 79.587 1.00 56.75	C
ATOM	5837 N SER D 317	20.878 15.857 76.879 1.00 59.33	N
		21.985 14.964 76.529 1.00 60.63	С
ATOM	5839 C SER D 317	23.029 15.693 75.710 1.00 58.92	С
ATOM	5840 O SER D 317	24.220 15.563 75.947 1.00 59.22	0
		21.463 13.769 75.722 1.00 62.99	C
ATOM	5842 OG SER D 317	20.092 14.067 75.446 1.00 66.00	Ο
ATOM	5843 N ALA D 318	22,565 16,502 74,770 1,00 57,14	N
ATOM	5844 CA ALA D 318	23.496 17.287 73.969 1.00 55.70	С
ATOM	5845 C ALA D 318	24.400 18.069 74.923 1.00 55.38	C
		25.619 18.111 74.754 1.00 55.90	
ATOM	5847 CB ALA D 318	22.719 18.241 73.089 1.00 55.59	C
ATOM	5848 N LEU D 319	23.784 18.710 75.917 1.00 54.11	
		24.469 19.510 76.902 1.00 52.31	С
ATOM	5850 C LEUD 319	25.325 18.635 77.770 1.00 53.63	С
ATOM	5851 O LEUD 319	26.487 18.939 77.974 1.00 53.68	0
ATOM	5852 CB LEU D 319	23.447 20.269 77.728 1.00 50.38 22.730 21.396 76.981 1.00 48.85	C
ATOM	5853 CG LEU D 319	22.730 21.396 76.981 1.00 48.85	С
		21.761 22.043 77.948 1.00 48.88	C
		23.707 22.414 76.424 1.00 48.75	C
		24.790 17.509 78.221 1.00 55.98	N
		25.548 16.575 79.053 1.00 57.36	
ATOM	5858 C LEU D 320	26.763 16.093 78.304 1.00 60.13	С
ATOM	5859 O LEUD 320	27.824 15.833 78.843 1.00 62.13	O C
ATOM	5860 CB LEU D 320	24.641 15.409 79.440 1.00 56.38 23.973 15.674 80.783 1.00 56.64	C
	5862 CD1 LEU D 320	23.038 14.548 81.152 1.00 56.78	C
		25.048 15.937 81.831 1.00 56.47	C
	5863 CD2 LEU D 320 5864 N ASP D 321	26.669 15.954 77.004 1.00 63.24	N
	5865 CA ASP D 321	27.748 15.558 76.161 1.00 66.90	C
	5866 C ASP D 321	28,809 16,606 75,920 1.00 66.24	C
	5867 O ASP D 321	29.986 16.236 75.844 1.00 68.96	Ö
	5868 CB ASP D 321	27.206 15.266 74.754 1.00 72.33	C
	5869 CG ASP D 321	27.150 13.752 74.641 1.00 77.63	Č
	5870 OD1 ASP D 321	27.464 13.085 75.664 1.00 80.31	0
	5871 OD2 ASP D 321	26.783 13.313 73.522 1.00 80.62	Ö
	5872 N ALA D 322	28.452 17.873 75.776 1.00 62.64	N
	5873 CA ALA D 322	29.463 18.891 75.524 1.00 58.96	C
	5874 C ALA D 322	30.353 19.113 76.735 1.00 58.25	C
	5875 O ALA D 322	31.386 19.785 76.571 1.00 58.76	0

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ATOM	5876 CB ALA D 322	28.714 20.137 75.123 1.00 57.92	C
		30.011 18.611 77.925 1.00 55.35	
ATOM	5878 CA GLUD 323	30.845 18.879 79.074 1.00 54.74	С
ATOM	5879 C GLU D 323	32.304 18.681 78.796 1.00 55.52	C
		32.712 17.725 78.133 1.00 59.31	0
ATOM	5881 CB GLUD 323	30.312 18.010 80.193 1.00 54.82	C C
ATOM	5882 CG GLUD 323	29.099 18.698 80.835 1.00 55.81	
ATOM	5883 CD GLUD 323	29.559 19.859 81.695 1.00 56.08 30.318 19.628 82.658 1.00 56.53	0
ATOM	5884 UEI GLU D 323	29.194 21.000 81.389 1.00 56.04	0
ATOM	5006 N DDO D 324	33.174 19.567 79.226 1.00 54.31	
ATOM	5887 CA PROD 324	34.603 19.489 79.046 1.00 53.97	C
ATOM	5888 C PRO D 324	35.190 18.524 80.065 1.00 54.99	C
		34.527 18.093 81.003 1.00 55.95	Ō
ATOM	5890 CB PRO D 324	35.145 20.897 79.323 1.00 53.50	С
ATOM	5891 CG PRO D 324	34.116 21.390 80.280 1.00 53.81	С
ATOM	5892 CD PRO D 324	34.116 21.390 80.280 1.00 53.81 32.788 20.736 80.013 1.00 54.57	С
ATOM	5893 N PRO D 325	36.446 18.172 79.897 1.00 55.53	N
ATOM	5894 CA PRO D 325	37.181 17.283 80.757 1.00 56.14	С
ATOM	5895 C PRO D 325	37.550 18.011 82.030 1.00 57.89	С
ATOM	5896 O PRO D 325	37.570 19.230 81.928 1.00 58.94	O
		38.475 16.991 79.994 1.00 56.36	
ATOM	5898 CG PRO D 325	38.641 18.258 79.193 1.00 56.53	C
ATOM	5899 CD PRO D 325	37.258 18.691 78.774 1.00 56.29	
ATOM	5900 N ILED 326	37.844 17.373 83.144 1.00 60.27	N C
		38.234 18.094 84.359 1.00 62.33 39.764 18.203 84.337 1.00 60.55	
ATOM	5902 C ILED 326	40.396 17.168 84.156 1.00 60.17	0
ATOM	5004 CB II E D 326	37.862 17.459 85.718 1.00 64.81	C
ATOM	5904 CB ILE D 326	38.409 16.036 85.871 1.00 66.11	C
		36.355 17.465 86.018 1.00 64.84	Č
		38.045 15.056 84.781 1.00 67.42	Č
		40.333 19.374 84.487 1.00 59.44	N
	5909 CA LEUD 327	41.786 19.485 84.472 1.00 58.05	С
	5910 C LEU D 327	42.321 19.216 85.865 1.00 58.59	С
ATOM	5911 O LEU D 327	41.603 19.137 86.848 1.00 58.48	0
ATOM	5912 CB LEU D 327	42.181 20.876 83.979 1.00 57.02	С
	5913 CG LEUD 327	41.514 21.360 82.693 1.00 55.77	С
	5914 CD1 LEU D 327	42.331 22.494 82.103 1.00 55.92	C
	5915 CD2 LEU D 327	41.316 20.258 81.683 1.00 54.67	C
	5916 N TYR D 328	43.625 19.048 85.975 1.00 60.29	N
	5917 CA TYR D 328	44.309 18.821 87.228 1.00 61.30	C
	5918 C TYR D 328	45.235 20.026 87.385 1.00 61.97	C O
	5919 O TYR D 328		C
ATOM	3920 CB 1 YK D 328	45.173 17.565 87.243 1.00 62.10	C

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ΔΤΟΜ	5921 CG TYR D 328	44.282 16.365 87.402 1.00 62.68	С
		43.836 16.059 88.678 1.00 64.19	
		43.876 15.593 86.339 1.00 62.75	
		42.988 15.002 88.813 1.00 64.91	С
		43.040 14.504 86.495 1.00 63.95	
		42.598 14.208 87.761 1.00 65.57	
		41.757 13.126 87.962 1.00 67.54	
		45.439 20.471 88.599 1.00 64.59	N
		46.299 21.612 88.807 1.00 67.29	
	5930 C SER D 329		C
		48.045 20.027 88.947 1.00 69.65	O C
		46.144 22.172 90.214 1.00 66.33 47.308 22.949 90.451 1.00 66.37	
		48.571 22.000 88.029 1.00 74.75	
ATOM	5935 CA GITID 330	49.973 21.777 87.782 1.00 78.76	C
		50.689 21.590 89.127 1.00 80.31	c
		50.542 22.260 90.146 1.00 80.76	
ATOM	5938 CB GLUD 330	50.572 22.972 87.056 1.00 82.49	C
ATOM	5939 CG GLUD 330	51.622 23.768 87.798 1.00 88.02	С
ATOM	5940 CD GLUD 330	51.312 25.158 88.310 1.00 91.02	С
ATOM	5941 OE1 GLU D 330	51.356 26.143 87.516 1.00 92.36	
		51.036 25.301 89.529 1.00 92.28	0
		52.571 28.436 99.492 1.00 85.53	N
		51.517 29.299 98.999 1.00 84.78	С
		51.805 30.749 99.360 1.00 83.45	
		51.984 31.023 100.540 1.00 84.23	
ATOM	5947 CB PHE D 337	50.138 28.994 99.593 1.00 85.69 49.414 27.933 98.825 1.00 86.82	C C
ATOM	5948 CG PHE D 337	49.414 27.933 98.823 1.00 80.82	C
		49.653 27.716 97.485 1.00 87.53 48.492 27.138 99.467 1.00 87.80	C
ATOM	5051 CELPHED 337	48.988 26.725 96.804 1.00 88.56	č
	5952 CE2 PHE D 337	47.808 26.143 98.802 1.00 88.39	Č
	5953 CZ PHE D 337	48.060 25.940 97.460 1.00 88.89	Č
	5954 N SER D 338	51.811 31.600 98.360 1.00 80.74	N
	5955 CA SER D 338	52.050 33.020 98.634 1.00 77.84	C
ATOM	5956 C SER D 338	51.096 33.751 97.717 1.00 75.96	C
ATOM	5957 O SER D 338	50.725 33.148 96.709 1.00 76.63	O
	5958 CB SER D 338	53.489 33.358 98.294 1.00 77.31	С
	5959 OG SER D 338	53.793 32.794 97.042 1.00 77.40	0
	5960 N GLUD 339	50.740 34.984 97.978 1.00 73.50	N
	5961 CA GLUD 339	49.848 35.681 97.047 1.00 71.53	C
	5962 C GLUD 339	50.264 35.297 95.634 1.00 69.88	C .
	5963 O GLUD 339	49.482 34.729 94.879 1.00 69.90 49.905 37.153 97.342 1.00 71.56	O C
	5964 CB GLU D 339 5965 CG GLU D 339	49.622 38.158 96.250 1.00 72.26	C
A I OIVI	2902 CG GLU D 339	47.022 30.130 90.230 1.00 /2.20	C

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4 TO 1 4	5066 CD CILID 220	49.019 39.364 96.939 1.00 73.84	С
ATOM	5967 OFI GUID 339	48.099 39.104 97.747 1.00 74.71	0
ATOM	5968 OE2 GLU D 339	49.466 40.503 96.691 1.00 75.27	Ö
		51.503 35.551 95.251 1.00 68.32	
ATOM	5970 CA ALAD 340	51.964 35.211 93.926 1.00 66.84	С
ATOM	5971 C ALA D 340	51.857 33.743 93.572 1.00 65.40	С
		51.426 33.462 92.464 1.00 65.53	
		53.428 35.594 93.817 1.00 68.19	
		52.278 32.843 94.438 1.00 64.29	
		52.224 31.429 94.117 1.00 63.99	
		50.790 30.981 93.942 1.00 63.79	
ATOM	5977 O SER D 341	50.499 30.238 92.997 1.00 65.43	0
ATOM	5978 CB SER D 341	52.954 30.602 95.145 1.00 65.29 52.117 20.756 05.800 1.00.66.80	C
A I UM	39/9 OG SERD 341	32.117 29.730 93.890 1.00 00.80	U
		49.868 31.390 94.800 1.00 62.43 48.477 31.005 94.670 1.00 60.24	
		48.477 31.003 94.670 1.00 60.24 47.790 31.641 93.472 1.00 58.97	
		47.111 30.947 92.714 1.00 60.15	
		47.632 31.381 95.885 1.00 60.40	
ATOM	5985 CG MET D 342	46.340 30.569 95.771 1.00.60.77	С
ATOM	5986 SD MET D 342	45.537 30.453 97.364 1.00 61.98 45.044 32.154 97.570 1.00 61.13	S
ATOM	5987 CE MET D 342	45.044 32.154 97.570 1.00 61.13	C
		47.943 32.936 93.235 1.00 56.72	
		47.372 33.564 92.053 1.00 54.94	
		47.886 32.813 90.835 1.00 54.84	
		47.107 32.531 89.932 1.00 56.41	0
		47.725 35.027 91.899 1.00 54.20	
		46.877 35.829 92.890 1.00 54.05	
ATOM	5994 SD MET D 343	45.115 35.671 92.551 1.00 51.49 45.079 35.840 90.775 1.00 52.48	S
	5995 CE MET D 343 5996 N GLY D 344		
		49.655 31.667 89.709 1.00 52.12	N C
		48.854 30.395 89.497 1.00 52.12	c
		48.396 30.211 88.372 1.00 52.11	Ö
		48.658 29.497 90.457 1.00 51.64	N
	6001 CA LEU D 345	47.931 28.273 90.199 1.00 52.00	C
	6002 C LEU D 345	46.528 28.472 89.651 1.00 51.27	С
ATOM	6003 O LEU D 345	46.087 27.901 88.665 1.00 51.16	0
ATOM	6004 CB LEU D 345	47.632 27.522 91.490 1.00 54.64	С
		48.809 26.826 92.152 1.00 57.14	С
		48.899 27.410 93.558 1.00 58.00	C
		48.609 25.316 92.126 1.00 57.34	C
	6008 N LEU D 346	45.815 29.290 90.432 1.00 49.48	N
	6009 CA LEUD 346	44.426 29.633 90.113 1.00 46.93	C
ATOM	6010 C LEUD 346	44.321 30.166 88.701 1.00 45.54	С

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ATOM	6011	O LEU D 346	43.616 29.725 87.814 1.00 43.40	0
ATOM	6012	CB LEU D 346	44.053 30.607 91.219 1.00 46.39	С
			43.730 29.934 92.553 1.00 46.28	С
			42.954 30.921 93.427 1.00 47.05	С
		CD2 LEU D 346	42,957 28,648 92,439 1.00 44.06	С
ATOM			45.136 31.171 88.432 1.00 45.12	N
			45.245 31.813 87.130 1.00 44.75	С
			45.663 30.858 86.058 1.00 44.99	C
ATOM	6019	O THR D 347	45.116 30.886 84.965 1.00 46.02	O
ATOM			46.194 32.989 87.399 1.00 44.97	C
ATOM			45.363 34.166 87.260 1.00 46.54	C
			47.482 32.992 86.660 1.00 43.19	Č
			46.589 29.951 86.286 1.00 45.79	N
ATOM			47.047 28.979 85.323 1.00 46.24	C
			45.907 28.023 85.019 1.00 45.11	c
			45.584 27.686 83.891 1.00 46.36	Ö
			48.233 28.214 85.903 1.00 49.70	Č
			48.707 27.068 85.007 1.00 53.34	Č
ATOM			48.323 25.881 85.136 1.00 54.22	0
			45.231 27.538 86.040 1.00 43.17	N
		CA LEU D 349		Ċ
			43.062 27.234 85.022 1.00 41.05	c
			42.587 26.634 84.073 1.00 41.06	0
			43.656 26.169 87.257 1.00 41.42	C
			42.504 25.188 87.265 1.00 41.73	C
ATOM		CD1 LEU D 349	42.911 23.883 86.597 1.00 42.98	С
ATOM			41.988 24.925 88.660 1.00 42.12	С
		N ALAD 350	•	N
			41.727 29.251 84.530 1.00 40.49	С
ATOM			42.117 29.313 83.060 1.00 40.66	С
			41.367 28.953 82.161 1.00 39.77	O
			41.615 30.689 85.022 1.00 39.66	С
		N ASP D 351	43.347 29.758 82.819 1.00 41.67	N
ATOM		CA ASP D 351	43.826 29.852 81.455 1.00 43.72	. C
		C ASP D 351	43.624 28.553 80.702 1.00 44.04	С
		O ASP D 351	43,309 28,530 79,516 1,00 44,68	0
		CB ASP D 351	45,277 30.315 81.445 1.00 46.16	C
ATOM		CG ASP D 351	45.749 30.472 80.006 1.00 49.30	С
ATOM		OD1 ASP D 351	45,392 31,418 79,275 1,00 50,41	0
		OD2 ASP D 351	46.520 29.592 79.570 1.00 51.19	0
		N ARG D 352	43.819 27.406 81.324 1.00 44.03	N
ATOM		CA ARG D 352	43.670 26.124 80.674 1.00 44.01	C
		C ARG D 352	42.236 25.737 80.426 1.00 44.62	С
		O ARG D 352	41.877 25.232 79.361 1.00 44.95	0
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ATOM	6056 CB ARG D 352	44.393 25.123 81.542 1.00 44.71	С
ATOM	6057 CG ARG D 352	45.899 25.219 81.311 1.00 45.89	С
ATOM	6058 CD ARG D 352	46.400 23.761 81.449 1.00 47.71	С
		46.531 23.597 82.889 1.00 50.31	
ATOM	6060 CZ ARG D 352	46.114 22.564 83.619 1.00 50.39	С
ATOM	6061 NH1 ARG D 352	45.535 21.583 82.950 1.00 49.57	N
		46.380 22.717 84.914 1.00 50.10	N
	6063 N GLUD 353		
		39.923 25.680 81.195 1.00 43.30	C C
		39.313 26.527 80.081 1.00 43.03 38.349 26.140 79.421 1.00 43.08	
		39.159 25.986 82.467 1.00 42.61	
		39.784 25.428 83.731 1.00 43.36	
ATOM	6069 CD GLUD 353	38.795 25.481 84.878 1.00 43.75	Č
		37.708 24.897 84.813 1.00 43.47	
		39.087 26.148 85.880 1.00 45.48	
		39.872 27.713 79.843 1.00 42.10	N
ATOM	6073 CA LEU D 354	39.372 28.627 78.849 1.00 41.53	С
		39,414 27.990 77.488 1.00 41.63	
		38.515 28.146 76.668 1.00 41.52	
ATOM	6076 CB LEU D 354	40.124 29.967 78.893 1.00 41.46	
		39.490 30.887 79.963 1.00 40.08	C
		40.509 31.876 80.452 1.00 39.39	
		38.254 31.514 79.349 1.00 39.73 40.476 27.242 77.253 1.00 42.96	N
		40.602 26.533 75.952 1.00 43.04	C
		39.447 25.551 75.825 1.00 43.28	
		38.664 25.632 74.882 1.00 43.52	
ATOM	6084 CB VALD 355	41 952 25 809 75 905 1 00 40 76	С
ATOM	6085 CG1 VAL D 355	42.078 24.985 74.684 1.00 40.05	С
ATOM	6086 CG2 VAL D 355	42.987 26.919 75.932 1.00 42.11	С
ATOM	6087 N HIS D 356	39.302 24.678 76.814 1.00 42.64	N
	6088 CA HIS D 356	38.199 23.750 76.794 1.00 44.51	С
	6089 C HIS D 356	36.873 24.475 76.676 1.00 43.62	C
	6090 O HIS D 356	35.992 24.023 75.945 1.00 42.64	0
	6091 CB HIS D 356	38.278 22.894 78.084 1.00 48.27	C C
	6092 CG HIS D 356	39.531 22.091 77.914 1.00 51.20 39.548 20.794 77.478 1.00 53.46	N
	6093 ND1 HIS D 356 6094 CD2 HIS D 356	40.812 22.436 78.082 1.00 52.88	C
	6095 CE1 HIS D 356	40.802 20.377 77.407 1.00 53.64	Č
	6096 NE2 HIS D 356	41.603 21.351 77.765 1.00 53.38	N
	6097 N MET D 357	36.716 25.583 77.406 1.00 43.17	N
	6098 CA MET D 357	35.488 26.349 77.384 1.00 42.35	С
	6099 C MET D 357	34.999 26.734 75.986 1.00 42.06	С
ATOM	6100 O MET D 357	33.834 26.548 75.656 1.00 41.73	Ο

WO 98/56812		12	245/371	PCT/GB98/01708
ATOM	6101	CB MET D 357	35.567 27.657 78.176 1.00 41.83	С
ATOM	6102	CG MET D 357	34.132 28.202 78.315 1.00 40.99	C
ATOM	6103	SD MET D 357	34.132 28.202 78.315 1.00 40.99 34.234 29.774 79.153 1.00 42.14	S
ATOM	6104	CE MET D 357	34.653 29.240 80.819 1.00 42.38	С
ATOM	6105	N ILE D 358	35.905 27.296 75.206 1.00 40.92	N
ATOM	6106	CA ILE D 358	35.618 27.703 73.852 1.00 40.82	С
ATOM	6107	C ILE D 358	35.088 26.509 73.082 1.00 42.56	С
ATOM	6108	O ILE D 358	34.088 26.641 72.391 1.00 43.58	0
ATOM	6109	CB ILE D 358	36.884 28.228 73.142 1.00 39.59	С
ATOM	6110	CG1 ILE D 358	37.398 29.499 73.829 1.00 39.34	С
ATOM	6111	CG2 ILE D 358	36.613 28.503 71.697 1.00 37.65	С
ATOM	6112	CD1 ILE D 358	38.667 30.064 73.264 1.00 37.60	С
			35.726 25.354 73.180 1.00 44.35	
ATOM	6114	CA ASN D 359	35.250 24.164 72.492 1.00 46.30	C
ATOM	6115	C ASN D 359	33.843 23.838 72.928 1.00 45.64	C
ATOM	6116	O ASN D 359	32.962 23.631 72.124 1.00 47.13	0
ATOM	6117	CB ASN D 359	36.155 22.978 72.842 1.00 51.34	C
ATOM	6118	CG ASN D 359	37.410 23.123 72.004 1.00 55.99	C
ATOM	6119	OD1 ASN D 359	37.180 23.150 70.781 1.00 60.17	0
ATOM	6120	ND2 ASN D 359	38.629 23.238 72.519 1.00 57.16	N
ATOM	6121	N TRP D 360	33.592 23.787 74.225 1.00 44.26	N
ATOM	6122	CA TRP D 360	32.296 23.479 74.769 1.00 41.88	C
ATOM	6123	C TRP D 360	31.234 24.400 74.223 1.00 41.73	С
ATOM	6124	O TRP D 360	30.110 24.054 73.906 1.00 40.64	0
ATOM	6125	CB TRP D 360	32.435 23.694 76.275 1.00 41.45	C
ATOM	6126	CG TRP D 360	31.082 23.808 76.915 1.00 41.81	C
ATOM	6127	CD1 TRP D 360	30.221 22.791 77.184 1.00 41.25 30.441 25.022 77.348 1.00 41.31	C
ATOM	6128	VEL TRR D 360	30.441 25.022 77.348 1.00 41.31	N
ATOM	6129	CE2 TRR D 360	29.095 23.305 77.750 1.00 41.05 29.198 24.657 77.871 1.00 40.99	C
ATOM	6130	CE2 TRP D 360	30.812 26.369 77.330 1.00 40.72	Č
ATOM	6137	CZ2 TRP D 360	28.311 25.581 78.398 1.00 41.54	Č
		CZ3 TRP D 360	29.928 27.279 77.843 1.00 41.39	Č
		CH2 TRP D 360	28.691 26.888 78.374 1.00 41.92	Č
		N ALA D 361	31.562 25.689 74.162 1.00 43.48	N
		CA ALA D 361	30.634 26.720 73.713 1.00 43.83	C
		C ALA D 361	30.132 26.330 72.341 1.00 45.28	С
		O ALA D 361	28.942 26.476 72.114 1.00 46.11	Ο
		CB ALA D 361	31.264 28.101 73.696 1.00 42.45	С
		N LYS D 362	30.980 25.849 71.446 1.00 46.93	N
		CA LYS D 362	30.618 25.471 70.112 1.00 48.98	С
		C LYS D 362	29.581 24.390 70.069 1.00 50.09	С
		O LYS D 362	28.874 24.303 69.074 1.00 52.06	o `
		CB LYS D 362	31.864 25.075 69.323 1.00 51.99	С
		CG LYS D 362	32.778 26.268 69.066 1.00 56.03	С
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WO 98/56812		246/371	PCT/GB98/01708
ATOM	6146 CD IVS D 362	32.135 27.218 68.051 1.00 60.32	С
ATOM	6147 CF LYS D 362	33.091 27.700 66.948 1.00 62.47	Č
ATOM	6148 NZ LYS D 362	32.412 28.297 65.742 1.00 62.21	N
		29.375 23.554 71.047 1.00 51.12	
ATOM	6150 CA ARG D 363	28.374 22.527 71.110 1.00 52.21	С
		27.113 22.909 71.852 1.00 50.20	
ATOM	6152 O ARG D 363	26.246 22.058 71.973 1.00 51.12	0
ATOM	6153 CB ARG D 363	28,935 21,320 71,868 1.00 56.54	С
ATOM	6154 CG ARG D 363	30.449 21.450 71.987 1.00 62.78 31.016 20.809 70.713 1.00 68.87	С
ATOM	6155 CD ARG D 363	31.016 20.809 70.713 1.00 68.87	С
ATOM	6156 NE ARG D 363	30.663 19.376 70.831 1.00 74.34	N
ATOM	6157 CZ ARG D 363	31.277 18.626 71.761 1.00 77.66	C
ATOM	6158 NH1 ARG D 363	32.203 19.186 72.544 1.00 78.42	N
		30.933 17.335 71.872 1.00 79.28	
ATOM	6160 N VAL D 364	26.934 24.079 72.396 1.00 48.90	N
		25.685 24.397 73.104 1.00 47.37	
ATOM	6162 C VAL D 364	24.686 24.663 72.004 1.00 46.99	С
ATOM	6163 O VAL D 364	24.855 25.578 71.218 1.00 47.63	O C
ATOM	6164 CB VAL D 364	25.869 25.635 74.003 1.00 45.65	C
ATOM	6165 CG1 VAL D 364	24.562 26.184 74.492 1.00 44.21 26.780 25.277 75.152 1.00 46.04	
			N
ATOM	6167 IN PROD 303	23.659 23.876 71.871 1.00 47.02 22.645 24.048 70.834 1.00 47.31	
		22.264 25.497 70.636 1.00 47.53	
ATOM	6170 O PRO D 365	21.941 26.186 71.590 1.00 49.08	Ō
		21.458 23.181 71.282 1.00 46.59	
		22.261 22.071 71.950 1.00 47.00	
ATOM	6173 CD PRO D 365	23.391 22.717 72.730 1.00 46.75	С
ATOM	6174 N GLY D 366	22.317 26.019 69.422 1.00 47.41	N
ATOM	6175 CA GLY D 366	21.964 27.385 69.106 1.00 46.04	С
	6176 C GLY D 366	23.122 28.343 69.012 1.00 45.85	С
		23.086 29.339 68.291 1.00 46.68	0
		24.190 28.083 69.738 1.00 45.21	N
		25.366 28.929 69.788 1.00 45.52	C
	6180 C PHE D 367	25.976 29.319 68.453 1.00 45.11	C
	6181 O PHE D 367	26.221 30.434 68.001 1.00 43.49	0
	6182 CB PHE D 367	26.477 28.279 70.656 1.00 44.32	C
		27.551 29.268 70.999 1.00 44.55	C
		27.363 30.300 71.898 1.00 44.50	C C
		28.773 29.162 70.366 1.00 45.53	C
		28.369 31.197 72.186 1.00 45.11 29.789 30.061 70.658 1.00 46.26	
		29.604 31.087 71.571 1.00 45.31	C
	6189 N VAL D 368	26.265 28.243 67.744 1.00 46.20	N N
		26.895 28.245 66.435 1.00 46.66	C
ATOM	0130 CV AVED 300	20.073 20.233 00.333 1.00 40.00	•

ATOM 6191 C VAL D 368	WO 98/56812		12	247/371	PCT/GB98/01708
ATOM 6192 O VAL D 368 ATOM 6193 CB VAL D 368 ATOM 6194 CGI VAL D 368 ATOM 6195 CG2 VAL D 368 ATOM 6195 CG2 VAL D 368 ATOM 6195 CG2 VAL D 368 ATOM 6196 N ASP D 369 ATOM 6197 CA ASP D 369 ATOM 6198 C ASP D 369 ATOM 6199 O ASP D 369 ATOM 6200 CB ASP D 369 ATOM 6201 CG ASP D 369 ATOM 6201 CG ASP D 369 ATOM 6202 OD1 ASP D 369 ATOM 6203 OD2 ASP D 369 ATOM 6203 OD2 ASP D 369 ATOM 6204 N LEU D 370 ATOM 6205 CA LEU D 370 ATOM 6206 C LEU D 370 ATOM 6207 CD LEU D 370 ATOM 6210 CD1 LEU D 370 ATOM 6211 CD2 LEU D 370 ATOM 6212 N THR D 371 ATOM 6213 CA THR D 371 ATOM 6213 CA THR D 371 ATOM 6216 CB THR D 371 ATOM 6217 CG1 THR D 371 ATOM 6218 CG2 THR D 371 ATOM 6210 CD LEU D 370 ATOM 6212 C LEU D 370 ATOM 6212 C LEU D 370 ATOM 6213 CA THR D 371 ATOM 6214 C THR D 371 ATOM 6215 CA LEU D 370 ATOM 6216 CB THR D 371 ATOM 6217 CG1 THR D 371 ATOM 6218 CG2 THR D 371 ATOM 6210 CD LEU D 370 ATOM 6210 CD LEU D 370 ATOM 6212 C LEU D 370 ATOM 6213 CA THR D 371 ATOM 6214 C THR D 371 ATOM 6215 CD LEU D 370 ATOM 6216 CB THR D 371 ATOM 6217 CG1 THR D 371 ATOM 6218 CG2 THR D 371 ATOM 6210 CD LEU D 370 ATOM 6210 CD LEU D 370 ATOM 6211 CD LEU D 370 ATOM 6212 C LEU D 370 ATOM 6213 CA THR D 371 ATOM 6214 C THR D 371 ATOM 6216 CB THR D 371 ATOM 6217 CG1 THR D 371 ATOM 6218 CG2 THR D 371 ATOM 6210 CD LEU D 372 ATOM 6220 C A LEU D 372 ATOM 6221 C LEU D 372 ATOM 6221 C LEU D 372 ATOM 6222 C LEU D 372 ATOM 6222 C LEU D 372 ATOM 6226 CD2 LEU D 372 ATOM 6227 N HIS D 373 ATOM 6228 CA HIS D 373 ATOM 6228 CA HIS D 373 ATOM 6229 C HIS D 373 ATOM 6229 C HIS D 373 ATOM 6220 C HIS D 373 ATOM 62	ATOM	6191	C VAL D 368		C
ATOM 6193 CB VAL D 368 ATOM 6194 CG1 VAL D 368 ATOM 6195 CG2 VAL D 368 ATOM 6195 CG2 VAL D 368 ATOM 6196 N ASP D 369 ATOM 6197 CA ASP D 369 ATOM 6198 C ASP D 369 ATOM 6199 O ASP D 369 ATOM 6200 CB ASP D 369 ATOM 6201 CG ASP D 369 ATOM 6201 CG ASP D 369 ATOM 6202 OD1 ASP D 369 ATOM 6202 OD1 ASP D 369 ATOM 6203 OD2 ASP D 369 ATOM 6204 N LEU D 370 ATOM 6205 CA LEU D 370 ATOM 6206 C LEU D 370 ATOM 6208 CB LEU D 370 ATOM 6209 CG LEU D 370 ATOM 6211 CD2 LEU D 370 ATOM 6212 N THR D 371 ATOM 6213 CA THR D 371 ATOM 6215 O THR D 371 ATOM 6216 CB THR D 371 ATOM 6216 CB THR D 371 ATOM 6217 OG1 THR D 371 ATOM 6218 CG2 THR D 371 ATOM 6220 CA LEU D 370 ATOM 6220 CA LEU D 370 ATOM 6212 C LEU D 370 ATOM 6213 CA THR D 371 ATOM 6214 C THR D 371 ATOM 6215 O THR D 371 ATOM 6216 CB THR D 371 ATOM 6217 OG1 THR D 371 ATOM 6218 CG2 THR D 371 ATOM 6219 N LEU D 372 ATOM 6220 CA LEU D 372 ATOM 6220 CA LEU D 372 ATOM 6221 C LEU D 372 ATOM 6222 O LEU D 372 ATOM 6222 CA LEU D 372 ATOM 6222 CA LEU D 372 ATOM 6222 CB LEU D 372 ATOM 6224 CG LEU D 372 ATOM 6225 CD1 LEU D 373 ATOM 6226 CD2 LEU D 373 ATOM 6227 N HIS D 373 ATOM 6228 CA HIS D 373 ATOM 6229 C HIS D 373 ATOM 6220 C					
ATOM 6194 CG1 VAL D 368 ATOM 6195 CG2 VAL D 368 ATOM 6196 N ASP D 369 ATOM 6197 CA ASP D 369 ATOM 6198 C ASP D 369 ATOM 6198 C ASP D 369 ATOM 6199 O ASP D 369 ATOM 6200 CB ASP D 369 ATOM 6200 CB ASP D 369 ATOM 6201 CG ASP D 369 ATOM 6202 OD1 ASP D 369 ATOM 6203 OD2 ASP D 369 ATOM 6203 OD2 ASP D 369 ATOM 6204 N LEU D 370 ATOM 6205 CA LEU D 370 ATOM 6206 C LEU D 370 ATOM 6207 O LEU D 370 ATOM 6207 O LEU D 370 ATOM 6201 CD1 LEU D 370 ATOM 6201 CD1 LEU D 370 ATOM 6202 CD1 LEU D 370 ATOM 6203 CA THR D 371 ATOM 6211 CD2 LEU D 370 ATOM 6212 N THR D 371 ATOM 6212 C THR D 371 ATOM 6216 CB THR D 371 ATOM 6216 CB THR D 371 ATOM 6216 CB THR D 371 ATOM 6212 C LEU D 370 ATOM 6215 O THR D 371 ATOM 6216 CB THR D 371 ATOM 6216 CB THR D 371 ATOM 6212 C LEU D 370 ATOM 6220 C LEU D 370 ATOM 6212 C LEU D 370 ATOM 6215 O THR D 371 ATOM 6216 CB THR D 371 ATOM 6217 CG2 THR D 371 ATOM 6218 CG2 THR D 371 ATOM 6219 N LEU D 372 ATOM 6220 CA LEU D 372 ATOM 6221 C LEU D 372 ATOM 6222 C LEU D 372 ATOM 6222 C LEU D 372 ATOM 6223 CB LEU D 372 ATOM 6224 CG LEU D 372 ATOM 6225 CD1 LEU D 373 ATOM 6226 CD2 LEU D 373 ATOM 6226 CD2 LEU D 372 ATOM 6227 N HIS D 373 ATOM 6228 CA HIS D 373 ATOM 6228 CA HIS D 373 ATOM 6229 C HIS D 373 ATOM 6220 CA HIS D 373 ATOM 6220 CHIS D 373 ATOM 6220 CA HIS D 373 ATOM 6220 CHIS D 373 ATOM 6220					С
ATOM 6195 CG2 VAL D 368 ATOM 6196 N ASP D 369 ATOM 6197 CA ASP D 369 ATOM 6198 C ASP D 369 ATOM 6199 O ASP D 369 ATOM 6199 O ASP D 369 ATOM 6200 CB ASP D 369 ATOM 6201 CG ASP D 369 ATOM 6201 CG ASP D 369 ATOM 6202 OD1 ASP D 369 ATOM 6202 OD1 ASP D 369 ATOM 6203 OD2 ASP D 369 ATOM 6204 N LEU D 370 ATOM 6205 CA LEU D 370 ATOM 6206 C LEU D 370 ATOM 6207 O LEU D 370 ATOM 6207 O LEU D 370 ATOM 6208 CB LEU D 370 ATOM 6211 CD2 LEU D 370 ATOM 6211 CD2 LEU D 370 ATOM 6212 N THR D 371 ATOM 6215 O THR D 371 ATOM 6216 CB THR D 371 ATOM 6216 CB THR D 371 ATOM 6217 CG1 THR D 371 ATOM 6218 CG2 THR D 371 ATOM 6220 C LEU D 370 ATOM 6210 CD LEU D 370 ATOM 6211 CD2 LEU D 370 ATOM 6212 N THR D 371 ATOM 6215 O THR D 371 ATOM 6216 CB THR D 371 ATOM 6216 CB THR D 371 ATOM 6217 CG1 THR D 371 ATOM 6218 CG2 THR D 371 ATOM 6210 CLEU D 370 ATOM 6210 CD THR D 371 ATOM 6211 CD2 LEU D 370 ATOM 6212 N THR D 371 ATOM 6214 C THR D 371 ATOM 6215 O THR D 371 ATOM 6216 CB THR D 371 ATOM 6216 CB THR D 371 ATOM 6217 CG1 THR D 371 ATOM 6218 CG2 THR D 371 ATOM 6220 CA LEU D 372 ATOM 6221 C LEU D 372 ATOM 6222 C LEU D 372 ATOM 6223 CB LEU D 372 ATOM 6224 CG LEU D 372 ATOM 6225 CD1 LEU D 373 ATOM 6226 CD2 LEU D 372 ATOM 6227 N HIS D 373 ATOM 6228 CA HIS D 373 ATOM 6228 CA HIS D 373 ATOM 6229 C HIS D 373 ATOM 6220 C HIS D 373 ATOM 6220 CA HIS D 373 ATOM 6220 CHIS D 372 ATOM 6220 CHIS D 373 ATOM 6220 CHIS					С
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ATOM 6201 CG ASP D 369	ATOM	6198	C ASP D 369	24.220 31.395 64.840 1.00 46.53	C
ATOM 6201 CG ASP D 369	ATOM	6199	O ASP D 369	23.595 32.145 64.116 1.00 47.73	0
ATOM 6202 OD1 ASP D 369 ATOM 6203 OD2 ASP D 369 ATOM 6204 N LEU D 370 ATOM 6205 CA LEU D 370 ATOM 6206 C LEU D 370 ATOM 6206 C LEU D 370 ATOM 6207 O LEU D 370 ATOM 6208 CB LEU D 370 ATOM 6209 CG LEU D 370 ATOM 6210 CD1 LEU D 370 ATOM 6211 CD2 LEU D 370 ATOM 6213 CA THR D 371 ATOM 6214 C THR D 371 ATOM 6215 O THR D 371 ATOM 6216 CB THR D 371 ATOM 6217 OG1 THR D 371 ATOM 6217 OG1 THR D 371 ATOM 6218 CG2 THR D 371 ATOM 6210 CD1 LEU D 370 ATOM 6211 CD2 LEU D 370 ATOM 6212 N THR D 371 ATOM 6213 CA THR D 371 ATOM 6214 C THR D 371 ATOM 6215 O THR D 371 ATOM 6216 CB THR D 371 ATOM 6217 OG1 THR D 371 ATOM 6218 CG2 THR D 371 ATOM 6219 N LEU D 372 ATOM 6210 CA LEU D 372 ATOM 6211 CD2 LEU D 372 ATOM 6217 OG1 THR D 371 ATOM 6218 CG2 THR D 371 ATOM 6219 N LEU D 372 ATOM 6210 CA LEU D 372 ATOM 6220 CA LEU D 372 ATOM 6221 C LEU D 372 ATOM 6221 C LEU D 372 ATOM 6221 C LEU D 372 ATOM 6222 O LEU D 372 ATOM 6224 CG LEU D 372 ATOM 6225 CD1 LEU D 372 ATOM 6226 CD2 LEU D 372 ATOM 6227 N HIS D 373 ATOM 6228 CA HIS D 373 ATOM 6228 CA HIS D 373 ATOM 6229 C HIS D 373 ATOM 6229 C HIS D 373 ATOM 6229 C HIS D 373 ATOM 6220 C HIS D 373	ATOM	6200	CB ASP D 369	22.469 29.720 65.013 1.00 52.83	C
ATOM 6203 OD2 ASP D 369 ATOM 6204 N LEU D 370 ATOM 6204 N LEU D 370 ATOM 6205 CA LEU D 370 ATOM 6206 C LEU D 370 ATOM 6207 O LEU D 370 ATOM 6208 CB LEU D 370 ATOM 6209 CG LEU D 370 ATOM 6210 CD1 LEU D 370 ATOM 6211 CD2 LEU D 370 ATOM 6212 N THR D 371 ATOM 6215 O THR D 371 ATOM 6216 CB THR D 371 ATOM 6216 CB THR D 371 ATOM 6217 OG1 THR D 371 ATOM 6218 CG2 THR D 371 ATOM 6219 CG LEU D 370 ATOM 6210 CD1 LEU D 370 ATOM 6211 CD2 LEU D 370 ATOM 6212 N THR D 371 ATOM 6213 CA THR D 371 ATOM 6214 C THR D 371 ATOM 6215 O THR D 371 ATOM 6216 CB THR D 371 ATOM 6217 OG1 THR D 371 ATOM 6218 CG2 THR D 371 ATOM 6219 C LEU D 372 ATOM 6220 CA LEU D 372 ATOM 6220 CA LEU D 372 ATOM 6221 C LEU D 372 ATOM 6220 CA LEU D 372 ATOM 6221 C LEU D 372 ATOM 6222 O LEU D 372 ATOM 6224 CG LEU D 372 ATOM 6255 CD1 LEU D 372 ATOM 6262 CD LEU D 372 ATOM 627 N HIS D 373 ATOM 628 CA HIS D 373 ATOM 629 C HIS D 373 ATOM 6228 CA HIS D 373 ATOM 6229 C HIS D 373 ATOM 6220 C HIS D 373	ATOM	6201	CG ASP D 369	22.039 28.271 64.957 1.00 57.29	C
ATOM 6204 N LEU D 370 ATOM 6205 CA LEU D 370 ATOM 6206 C LEU D 370 ATOM 6206 C LEU D 370 ATOM 6207 O LEU D 370 ATOM 6208 CB LEU D 370 ATOM 6208 CB LEU D 370 ATOM 6209 CG LEU D 370 ATOM 6210 CD1 LEU D 370 ATOM 6211 CD2 LEU D 370 ATOM 6212 N THR D 371 ATOM 6213 CA THR D 371 ATOM 6216 CB THR D 371 ATOM 6216 CB THR D 371 ATOM 6217 OG1 THR D 371 ATOM 6218 CG2 THR D 371 ATOM 6219 N LEU D 372 ATOM 6210 CB LEU D 372 ATOM 6210 CB THR D 371 ATOM 6211 CD2 LEU D 370 ATOM 6212 N THR D 371 ATOM 6213 CA THR D 371 ATOM 6214 C THR D 371 ATOM 6215 O THR D 371 ATOM 6216 CB THR D 371 ATOM 6217 OG1 THR D 371 ATOM 6218 CG2 THR D 371 ATOM 6219 N LEU D 372 ATOM 6220 CA LEU D 372 ATOM 6221 C LEU D 372 ATOM 6222 O LEU D 372 ATOM 6223 CB LEU D 372 ATOM 6224 CG LEU D 372 ATOM 625 CD1 LEU D 372 ATOM 626 CD2 LEU D 372 ATOM 626 CD2 LEU D 372 ATOM 627 N HIS D 373 ATOM 628 CA HIS D 373 ATOM 629 C HIS D 373 ATOM 6229 C HIS D 373 ATOM 6220 C HIS D 373	ATOM	6202	OD1 ASP D 369	22.549 27.486 64.111 1.00 59.44	0
ATOM 6205 CA LEU D 370	ATOM	6203	OD2 ASP D 309	21,100 27,927 03,791 1.00 39.33	N
ATOM 6206 C LEU D 370 ATOM 6207 O LEU D 370 ATOM 6208 CB LEU D 370 ATOM 6208 CB LEU D 370 ATOM 6209 CG LEU D 370 ATOM 6210 CD1 LEU D 370 ATOM 6211 CD2 LEU D 370 ATOM 6212 N THR D 371 ATOM 6213 CA THR D 371 ATOM 6216 CB THR D 371 ATOM 6216 CB THR D 371 ATOM 6217 OG1 THR D 371 ATOM 6218 CG2 THR D 371 ATOM 6219 N LEU D 372 ATOM 6210 CD LEU D 372 ATOM 6210 CD THR D 371 ATOM 6211 CD2 LEU D 370 ATOM 6212 N THR D 371 ATOM 6213 CA THR D 371 ATOM 6214 C THR D 371 ATOM 6215 O THR D 371 ATOM 6216 CB THR D 371 ATOM 6217 OG1 THR D 371 ATOM 6218 CG2 THR D 371 ATOM 6219 N LEU D 372 ATOM 6220 CA LEU D 372 ATOM 6221 C LEU D 372 ATOM 6221 C LEU D 372 ATOM 6222 O LEU D 372 ATOM 6224 CG LEU D 372 ATOM 6225 CD1 LEU D 372 ATOM 6226 CD2 LEU D 372 ATOM 6227 N HIS D 373 ATOM 6228 CA HIS D 373 ATOM 6229 C HIS D 373 ATOM 6220 C HIS D 373 ATOM 6220 C HIS D 373 ATOM 6228 CA HIS D 373 ATOM 6228 CA HIS D 373 ATOM 6229 C HIS D 373	ATOM	6204	CA LEUD 370	25.002 31.928 05.730 1.00 43.83	C
ATOM 6207 O LEU D 370 ATOM 6208 CB LEU D 370 ATOM 6209 CG LEU D 370 ATOM 6209 CG LEU D 370 ATOM 6210 CD1 LEU D 370 ATOM 6211 CD2 LEU D 370 ATOM 6212 N THR D 371 ATOM 6213 CA THR D 371 ATOM 6214 C THR D 371 ATOM 6215 O THR D 371 ATOM 6216 CB THR D 371 ATOM 6217 OG1 THR D 371 ATOM 6218 CG2 THR D 371 ATOM 6219 N LEU D 372 ATOM 6220 CA LEU D 372 ATOM 6220 CA LEU D 372 ATOM 6220 CE LEU D 372 ATOM 6221 C LEU D 372 ATOM 6220 CE LEU D 372 ATOM 6220 CE LEU D 372 ATOM 6221 C LEU D 372 ATOM 6222 O LEU D 372 ATOM 6223 CB LEU D 372 ATOM 6224 CG LEU D 372 ATOM 6225 CD1 LEU D 372 ATOM 6226 CD2 LEU D 373 ATOM 6227 N HIS D 373 ATOM 6228 CA HIS D 373 ATOM 6228 CA HIS D 373 ATOM 6229 C HIS D 373 ATOM 6229 C HIS D 373 ATOM 6229 C HIS D 373 ATOM 6220 C HIS D 373					
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ATOM 6210 CD1 LEU D 370 ATOM 6211 CD2 LEU D 370 ATOM 6212 N THR D 371 ATOM 6213 CA THR D 371 ATOM 6214 C THR D 371 ATOM 6215 O THR D 371 ATOM 6216 CB THR D 371 ATOM 6216 CB THR D 371 ATOM 6217 OG1 THR D 371 ATOM 6218 CG2 THR D 371 ATOM 6219 N LEU D 372 ATOM 6220 CA LEU D 372 ATOM 6221 C LEU D 372 ATOM 6222 O LEU D 372 ATOM 6225 CD1 LEU D 372 ATOM 6226 CD2 LEU D 373 ATOM 6227 N HIS D 373 ATOM 6227 N HIS D 373 ATOM 6228 CA HIS D 373 ATOM 6228 CA HIS D 373 ATOM 6229 C HIS D 373 ATOM 6229 C HIS D 373 ATOM 6220 C LEU D 372 ATOM 6220 CD LEU D 373 ATOM 6220 CD LEU D 373 ATOM 6220 CD HIS D 373	ATOM	6208	CB LEUD 370	25 482 33 706 67 325 1 00 44 43	
ATOM 6210 CD1 LEU D 370	ATOM	6209	CG LEUD 370	24 324 33 418 68 273 1 00 44 60	
ATOM 6211 CD2 LEU D 370 ATOM 6212 N THR D 371 ATOM 6213 CA THR D 371 ATOM 6213 CA THR D 371 ATOM 6214 C THR D 371 ATOM 6215 O THR D 371 ATOM 6216 CB THR D 371 ATOM 6217 OG1 THR D 371 ATOM 6218 CG2 THR D 371 ATOM 6219 N LEU D 372 ATOM 6210 CA LEU D 372 ATOM 6220 CA LEU D 372 ATOM 6221 C LEU D 372 ATOM 6222 O LEU D 372 ATOM 6223 CB LEU D 372 ATOM 6224 CG LEU D 372 ATOM 6226 CD2 LEU D 372 ATOM 6227 N HIS D 373 ATOM 6228 CA HIS D 373 ATOM 6229 C HIS D 373					
ATOM 6212 N THR D 371 26.573 35.055 64.634 1.00 41.97 N ATOM 6213 CA THR D 371 27.740 35.393 63.833 1.00 41.89 C ATOM 6214 C THR D 371 28.996 35.122 64.629 1.00 42.57 C ATOM 6215 O THR D 371 29.066 35.192 65.842 1.00 42.44 O ATOM 6216 CB THR D 371 27.753 36.867 63.472 1.00 42.11 C ATOM 6217 OG1 THR D 371 27.590 37.524 64.730 1.00 44.12 O ATOM 6218 CG2 THR D 371 26.588 37.224 62.583 1.00 42.85 C ATOM 6219 N LEU D 372 30.084 34.819 63.921 1.00 44.42 N ATOM 6220 CA LEU D 372 31.684 35.588 65.615 1.00 44.22 C ATOM 6221 C LEU D 372 31.684 35.588 65.615 1.00 45.55 C ATOM 6222 O LEU D 372 32.135 35.219 66.713 1.00 46.54 O ATOM 6223 CB LEU D 372 32.400 34.370 63.500 1.00 43.22 C ATOM 6224 CG LEU D 372 32.400 34.370 63.500 1.00 43.22 C ATOM 6225 CD1 LEU D 372 32.274 33.164 62.587 1.00 42.31 C ATOM 6226 CD2 LEU D 372 32.422 31.864 63.359 1.00 42.37 C ATOM 6227 N HIS D 373 31.476 36.879 65.357 1.00 45.87 N ATOM 6228 CA HIS D 373 31.821 37.871 66.364 1.00 46.42 C ATOM 6229 C HIS D 373 30.894 37.785 67.553 1.00 45.97 C	ATOM	6211	CD2 LEU D 370	23.174 34.327 67.868 1.00 45.07	
ATOM 6213 CA THR D 371 27.740 35.393 63.833 1.00 41.89 C ATOM 6214 C THR D 371 28.996 35.122 64.629 1.00 42.57 C ATOM 6215 O THR D 371 29.066 35.192 65.842 1.00 42.44 O ATOM 6216 CB THR D 371 27.753 36.867 63.472 1.00 42.11 C ATOM 6217 OG1 THR D 371 27.590 37.524 64.730 1.00 44.12 O ATOM 6218 CG2 THR D 371 26.588 37.224 62.583 1.00 42.85 C ATOM 6219 N LEU D 372 30.084 34.819 63.921 1.00 44.42 N ATOM 6220 CA LEU D 372 31.352 34.525 64.582 1.00 44.22 C ATOM 6221 C LEU D 372 31.684 35.588 65.615 1.00 45.55 C ATOM 6222 O LEU D 372 32.135 35.219 66.713 1.00 46.54 O ATOM 6223 CB LEU D 372 32.400 34.370 63.500 1.00 43.22 C ATOM 6224 CG LEU D 372 32.400 34.370 63.500 1.00 42.31 C ATOM 6225 CD1 LEU D 372 32.400 34.370 63.500 1.00 42.37 C ATOM 6226 CD2 LEU D 372 32.422 31.864 63.359 1.00 42.37 C ATOM 6227 N HIS D 373 31.476 36.879 65.357 1.00 45.87 N ATOM 6228 CA HIS D 373 31.821 37.871 66.364 1.00 46.42 C ATOM 6229 C HIS D 373 30.894 37.785 67.553 1.00 45.97 C					
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ATOM 6218 CG2 THR D 371 26.588 37.224 62.583 1.00 42.85 C ATOM 6219 N LEU D 372 30.084 34.819 63.921 1.00 44.42 N ATOM 6220 CA LEU D 372 31.352 34.525 64.582 1.00 44.22 C ATOM 6221 C LEU D 372 31.684 35.588 65.615 1.00 45.55 C ATOM 6222 O LEU D 372 32.135 35.219 66.713 1.00 46.54 O ATOM 6223 CB LEU D 372 32.400 34.370 63.500 1.00 43.22 C ATOM 6224 CG LEU D 372 32.274 33.164 62.587 1.00 42.31 C ATOM 6225 CD1 LEU D 372 33.405 33.206 61.575 1.00 42.31 C ATOM 6226 CD2 LEU D 372 32.422 31.864 63.359 1.00 43.20 C ATOM 6227 N HIS D 373 31.476 36.879 65.357 1.00 45.87 N ATOM 6228 CA HIS D 373 31.821 37.871 66.364 1.00 46.42 C ATOM 6229 C HIS D 373 30.894 37.785 67.553 1.00 45.97 C	ATOM	6216	CB THR D 371	27.753 36.867 63.472 1.00 42.11	
ATOM 6219 N LEU D 372 30.084 34.819 63.921 1.00 44.42 N ATOM 6220 CA LEU D 372 31.352 34.525 64.582 1.00 44.22 C ATOM 6221 C LEU D 372 31.684 35.588 65.615 1.00 45.55 C ATOM 6222 O LEU D 372 32.135 35.219 66.713 1.00 46.54 O ATOM 6223 CB LEU D 372 32.400 34.370 63.500 1.00 43.22 C ATOM 6224 CG LEU D 372 32.274 33.164 62.587 1.00 42.31 C ATOM 6225 CD1 LEU D 372 33.405 33.206 61.575 1.00 42.37 C ATOM 6226 CD2 LEU D 372 32.422 31.864 63.359 1.00 43.20 C ATOM 6227 N HIS D 373 31.476 36.879 65.357 1.00 45.87 N ATOM 6228 CA HIS D 373 31.821 37.871 66.364 1.00 46.42 C ATOM 6229 C HIS D 373 30.894 37.785 67.553 1.00 45.97 C					
ATOM 6220 CA LEU D 372 31.352 34.525 64.582 1.00 44.22 C ATOM 6221 C LEU D 372 31.684 35.588 65.615 1.00 45.55 C ATOM 6222 O LEU D 372 32.135 35.219 66.713 1.00 46.54 O ATOM 6223 CB LEU D 372 32.400 34.370 63.500 1.00 43.22 C ATOM 6224 CG LEU D 372 32.274 33.164 62.587 1.00 42.31 C ATOM 6225 CD1 LEU D 372 33.405 33.206 61.575 1.00 42.37 C ATOM 6226 CD2 LEU D 372 32.422 31.864 63.359 1.00 43.20 C ATOM 6227 N HIS D 373 31.476 36.879 65.357 1.00 45.87 N ATOM 6228 CA HIS D 373 31.821 37.871 66.364 1.00 46.42 C ATOM 6229 C HIS D 373 30.894 37.785 67.553 1.00 45.97 C					
ATOM 6221 C LEU D 372 31.684 35.588 65.615 1.00 45.55 C ATOM 6222 O LEU D 372 32.135 35.219 66.713 1.00 46.54 O ATOM 6223 CB LEU D 372 32.400 34.370 63.500 1.00 43.22 C ATOM 6224 CG LEU D 372 32.274 33.164 62.587 1.00 42.31 C ATOM 6225 CD1 LEU D 372 33.405 33.206 61.575 1.00 42.37 C ATOM 6226 CD2 LEU D 372 32.422 31.864 63.359 1.00 43.20 C ATOM 6227 N HIS D 373 31.476 36.879 65.357 1.00 45.87 N ATOM 6228 CA HIS D 373 31.821 37.871 66.364 1.00 46.42 C ATOM 6229 C HIS D 373 30.894 37.785 67.553 1.00 45.97 C	ATOM	6219	N LEU D 372	30.084 34.819 63.921 1.00 44.42	
ATOM 6222 O LEU D 372 32.135 35.219 66.713 1.00 46.54 O ATOM 6223 CB LEU D 372 32.400 34.370 63.500 1.00 43.22 C ATOM 6224 CG LEU D 372 32.274 33.164 62.587 1.00 42.31 C ATOM 6225 CD1 LEU D 372 33.405 33.206 61.575 1.00 42.37 C ATOM 6226 CD2 LEU D 372 32.422 31.864 63.359 1.00 43.20 C ATOM 6227 N HIS D 373 31.476 36.879 65.357 1.00 45.87 N ATOM 6228 CA HIS D 373 31.821 37.871 66.364 1.00 46.42 C ATOM 6229 C HIS D 373 30.894 37.785 67.553 1.00 45.97 C					
ATOM 6223 CB LEU D 372 32.400 34.370 63.500 1.00 43.22 C ATOM 6224 CG LEU D 372 32.274 33.164 62.587 1.00 42.31 C ATOM 6225 CD1 LEU D 372 33.405 33.206 61.575 1.00 42.37 C ATOM 6226 CD2 LEU D 372 32.422 31.864 63.359 1.00 43.20 C ATOM 6227 N HIS D 373 31.476 36.879 65.357 1.00 45.87 N ATOM 6228 CA HIS D 373 31.821 37.871 66.364 1.00 46.42 C ATOM 6229 C HIS D 373 30.894 37.785 67.553 1.00 45.97 C					
ATOM 6224 CG LEU D 372 32.274 33.164 62.587 1.00 42.31 C ATOM 6225 CD1 LEU D 372 33.405 33.206 61.575 1.00 42.37 C ATOM 6226 CD2 LEU D 372 32.422 31.864 63.359 1.00 43.20 C ATOM 6227 N HIS D 373 31.476 36.879 65.357 1.00 45.87 N ATOM 6228 CA HIS D 373 31.821 37.871 66.364 1.00 46.42 C ATOM 6229 C HIS D 373 30.894 37.785 67.553 1.00 45.97 C					
ATOM 6225 CD1 LEU D 372 33.405 33.206 61.575 1.00 42.37 C ATOM 6226 CD2 LEU D 372 32.422 31.864 63.359 1.00 43.20 C ATOM 6227 N HIS D 373 31.476 36.879 65.357 1.00 45.87 N ATOM 6228 CA HIS D 373 31.821 37.871 66.364 1.00 46.42 C ATOM 6229 C HIS D 373 30.894 37.785 67.553 1.00 45.97 C					
ATOM 6226 CD2 LEU D 372 32.422 31.864 63.359 1.00 43.20 C ATOM 6227 N HIS D 373 31.476 36.879 65.357 1.00 45.87 N ATOM 6228 CA HIS D 373 31.821 37.871 66.364 1.00 46.42 C ATOM 6229 C HIS D 373 30.894 37.785 67.553 1.00 45.97 C					
ATOM 6227 N HIS D 373 31.476 36.879 65.357 1.00 45.87 N ATOM 6228 CA HIS D 373 31.821 37.871 66.364 1.00 46.42 C ATOM 6229 C HIS D 373 30.894 37.785 67.553 1.00 45.97 C					
ATOM 6228 CA HIS D 373 31.821 37.871 66.364 1.00 46.42 C ATOM 6229 C HIS D 373 30.894 37.785 67.553 1.00 45.97 C					
ATOM 6229 C HIS D 373 30.894 37.785 67.553 1.00 45.97 C					
UT O171 A710 O 1117 21.210 21.210 21.275 00.002 1.00 42.02				31.376 37.912 68.685 1.00 45.63	0
ATOM 6231 CB HIS D 373 31.928 39.239 65.738 1.00 48.92 C				31.928 39.239 65.738 1.00 48.92	
ATOM 6232 CG HIS D 373 33.222 39.415 64.998 1.00 52.20 C	ATOM	6232	CG HIS D 373		
ATOM 6233 ND1 HIS D 373 33.327 39.410 63.612 1.00 54.08 N					
ATOM 6234 CD2 HIS D 373 34.483 39.619 65.412 1.00 52.17 C					
ATOM 6235 CE1 HIS D 373 34.585 39.608 63.254 1.00 53.36 C	ATOM	6235	CE1 HIS D 373	34.585 39.608 63.254 1.00 53.36	C

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,,,	,=		249/371	
ATOM		CG LEUD 378	26.947 35.482 73.233 1.00 40.01	С
		CD1 LEU D 378	25.938 34.407 72.906 1.00 39.46	C
		CD2 LEU D 378	26.289 36.641 73.989 1.00 40.25	С
		N LEU D 379	31.256 34.725 74.740 1.00 39.51	N
		CA LEU D 379	32.366 34.132 75.452 1.00 38.70	С
		C LEU D 379	33.070 35.171 76.293 1.00 38.95	C
		O LEU D 379	33.112 35.019 77.509 1.00 37.69	0
ATOM		CB LEU D 379	33.333 33.515 74.462 1.00 38.77	C
ATOM		CG LEU D 379	32.984 32.035 74.273 1.00 39.28	C
		_	33.914 31.556 73.159 1.00 40.30	C
		CD2 LEU D 379	33.061 31.264 75.581 1.00 37.03	С
		N GLUD 380	33.544 36.240 75.642 1.00 40.00	N
		CA GLUD 380	34.189 37.305 76.416 1.00 41.67	С
		C GLU D 380	33.284 37.785 77.545 1.00 43.10	С
		O GLU D 380	33.718 38.049 78.653 1.00 43.41	0
		CB GLUD 380	34.498 38.490 75.530 1.00 40.94	С
			35.532 38.158 74.456 1.00 43.88	C
		CD GLUD 380	35.639 39.372 73.551 1.00 46.53	C
		OE1 GLU D 380	34.609 40.105 73.396 1.00 48.71	0
		OE2 GLU D 380	36.732 39.604 73.006 1.00 47.01	0
ATOM		N CYS D 381	31.981 37.920 77.295 1.00 44.81	N
		CA CYS D 381		С
		C CYS D 381	30.987 37.415 79.488 1.00 43.56	C
		O CYS D 381	31.118 37.898 80.604 1.00 42.78	0
ATOM		CB CYS D 381	29.761 38.864 77.771 1.00 50.78	C
ATOM		SG CYS D 381	29.626 40.658 78.224 1.00 63.43	S
		N ALA D 382	30.743 36.138 79.292 1.00 41.65	N
		CA ALAD 382	30.518 35.213 80.385 1.00 40.09	C C
ATOM		C ALA D 382	31.613 34.307 80.877 1.00 39.58	_
		O ALA D 382	31.352 33.505 81.778 1.00 39.62	O C
		CB ALA D 382	29.399 34.303 79.819 1.00 38.89	N
		N TRP D 383	32.834 34.376 80.378 1.00 39.40 33.896 33.455 80.771 1.00 38.01	C
		CA TRP D 383	34,029 33,173 82.253 1.00 37.84	C
		C TRP D 383	33,935 32,027 82,709 1.00 37.84	o
		O TRP D 383	35.185 33.887 80.105 1.00 36.76	C
		CB TRP D 383	35.874 35.059 80.689 1.00 35.63	C
		CG TRP D 383	35.744 36.370 80.365 1.00 35.20	C
		CD1 TRP D 383	36.869 34.994 81.718 1.00 35.85	C
		CD2 TRP D 383 NE1 TRP D 383	36.573 37.127 81.145 1.00 33.83	N
		CE2 TRP D 383	37.275 36.306 81.987 1.00 34.93	C
			37.415 33.946 82.467 1.00 35.33	c
		CE3 TRP D 383	38,222 36.578 82.953 1.00 35.70	C
		CZ2 TRP D 383 CZ3 TRP D 383	38,348 34,254 83,432 1,00 35.86	C
		CH2 TRP D 383	38.756 35.549 83.663 1.00 35.16	C
AIUM	0323	CUT IKL D 393	30.750 27.003 1.00 33.10	C

WO 98/56812		20/371	PCT/GB98/01708
4 TO 1 4	6326 N LEUD 384	250/371 34.204 34.232 83.045 1.00 37.07	N
		34.361 34.073 84.485 1.00 34.29	C
ATOM	6327 CA LEU D 384	33.083 33.572 85.091 1.00 34.07	c
ATOM	6320 O I FII D 384	33.133 32.783 86.024 1.00 35.02	Ö
		34.950 35.349 85.060 1.00 33.01	C
ATOM	6331 CG LEUD 384	35.310 35.329 86.535 1.00 34.01	Ċ
ATOM	6332 CD1 LEU D 384	36.154 34.136 86.972 1.00 34.20	Ċ
ATOM	6333 CD2 LEU D 384	36.009 36.630 86.889 1.00 33.55	Č
	6334 N GLUD 385		N
	6335 CA GLUD 385		С
ATOM	6336 C GLU D 385	30.672 31.900 85.031 1.00 33.61	С
ATOM	6337 O GLUD 385	30.488 31.121 85.955 1.00 32.47	0
ATOM	6338 CB GLU D 385	29.414 34.058 84.678 1.00 34.46	С
ATOM	6339 CG GLU D 385	28.899 35.317 85.300 1.00 36.30	С
		27.712 35.900 84.551 1.00 39.20	С
		27.989 36.563 83.508 1.00 38.66	0
		26.516 35.719 84.973 1.00 40.99	0
		30.940 31.453 83.816 1.00 34.27	N
		31.023 30.042 83.501 1.00 35.57	С
ATOM	6345 C ILE D 386	32.051 29.353 84.403 1.00 36.46	С
ATOM	6346 O ILE D 386	31.753 28.302 84.965 1.00 36.26	0
		31.462 29.651 82.087 1.00 36.16	С
		30.810 30.376 80.921 1.00 38.67	С
ATOM	6349 CG2 ILE D 386	31.205 28.173 81.927 1.00 35.09	С
ATOM	6350 CD1 ILE D 386	29.305 30.310 80.872 1.00 40.67	C .
		33.274 29.877 84.553 1.00 37.57	N
		34.268 29.247 85.404 1.00 36.90	С
ATOM	6353 C LEUD 387	33.732 29.174 86.831 1.00 38.44	С
		33.820 28.105 87.468 1.00 40.27	0
		35.591 29.959 85.496 1.00 36.96	С
		36.524 29.891 84.290 1.00 38.44	С
ATOM	6357 CD1 LEU D 387	37.742 30.803 84.456 1.00 38.18	
		36.933 28.455 84.054 1.00 38.32	С
		33.149 30.263 87.336 1.00 37.63	N
		32.665 30.221 88.705 1.00 37.22	C
		31.539 29.252 88.906 1.00 38.19	C
	6362 O MET D 388		0
	6363 CB MET D 388		C
		33.246 32.708 89.036 1.00 38.43	C
		32.935 34.095 90.117 1.00 39.57	S
		34.516 34.928 90.147 1.00 40.10	C
	6367 N ILE D 389		N
		29.485 28.137 88.321 1.00 40.84	C
	6369 C ILE D 389		С
ATOM	6370 O ILE D 389	29.640 25.844 89.053 1.00 43.43	0

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АТОМ	6371 CB ILE D 389	28.247 28.326 87.427 1.00 37.94	С
ATOM	6372 CG1 ILE D 389	27.068 27.488 87.908 1.00 36.69	C
ATOM	6373 CG2 ILE D 389	27.068 27.488 87.908 1.00 36.69 28.622 27.941 86.030 1.00 36.39	C
ATOM	6374 CD1 ILE D 389	25.732 27.888 87.384 1.00 34.40	С
		31.076 26.487 87.474 1.00 41.93	
ATOM	6376 CA GLY D 390	31.680 25.159 87.421 1.00 42.20	С
		32.294 24.860 88.770 1.00 42.14	
		32.038 23.806 89.321 1.00 41.64	
ATOM	6379 N LEU D 391	33.068 25.848 89.246 1.00 42.56	N
ATOM	6380 CA LEU D 391	33.741 25.678 90.541 1.00 41.55	С
ATOM	6381 C LEUD 391	32.731 25.332 91.599 1.00 41.30	С
ATOM	6382 O LEU D 391	32.765 24.333 92.268 1.00 42.41	0
ATOM	6383 CB LEU D 391	34.471 26.946 90.967 1.00 40.77	С
ATOM	6384 CG LEU D 391	35.090 27.007 92.349 1.00 41.23	C
ATOM	6385 CD1 LEU D 391	35.090 27.007 92.349 1.00 41.23 36.095 25.868 92.543 1.00 41.69	C
ATOM	6386 CD2 LEU D 391	35.784 28.323 92.643 1.00 41.15	С
		31.757 26.194 91.775 1.00 42.54	
ATOM	6388 CA VAL D 392	30.712 26.047 92.770 1.00 42.50	C
		30.087 24.673 92.725 1.00 44.06	
		29.878 24.012 93.738 1.00 44.87	
		29.661 27.150 92.609 1.00 41.04	
ATOM	6392 CG1 VAL D 392	28.457 26.838 93.465 1.00 40.61	C
		30.233 28.468 93.091 1.00 40.68	
		29.749 24.233 91.530 1.00 45.63	
		29.106 22.954 91.287 1.00 46.45	
ATOM	6396 C TRP D 393	29.993 21.800 91.697 1.00 46.87	0
ATOM	6397 O TRP D 393	29.499 20.900 92.357 1.00 47.71 28.821 22.832 89.788 1.00 47.26	C
		28.626 21.413 89.360 1.00 47.45	
		29.474 20.649 88.625 1.00 47.21	C
ATOM	6401 CD2 TRP D 393	27.495 20.592 89.658 1.00 47.89	Č
	6402 NE1 TRP D 393	28.934 19.407 88.437 1.00 47.18	N
	6403 CE2 TRP D 393	27.722 19.336 89.057 1.00 47.38	C
	6404 CE3 TRP D 393	26.314 20.800 90.373 1.00 48.23	Č
	6405 CZ2 TRP D 393	26.821 18.281 89.148 1.00 47.14	C
	6406 CZ3 TRP D 393	25.423 19.753 90.471 1.00 48.58	С
	6407 CH2 TRP D 393	25.683 18.514 89.859 1.00 48.15	С
	6408 N ARG D 394	31.261 21.843 91.276 1.00 47.26	N
	6409 CA ARG D 394	32.153 20.755 91.647 1.00 47.47	С
ATOM	6410 C ARG D 394	32.522 20.880 93.110 1.00 48.85	С
	6411 O ARG D 394	32.965 19.910 93.710 1.00 51.34	0
ATOM	6412 CB ARG D 394	33.346 20.565 90.751 1.00 45.88	С
	6413 CG ARG D 394	34.195 21.670 90.285 1.00 45.23	С
	6414 CD ARG D 394	35.404 21.219 89.472 1.00 44.56	С
ATOM	6415 NE ARG D 394	36.333 22.366 89.420 1.00 44.88	N

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ATOM	6461 C GLY D 400	34.787 24.865 102.689 1.00 56.74	С
ATOM	6462 O GLY D 400	35.733 25.606 103.049 1.00 57.61	0
ATOM	6463 N LYS D 401	34.827 24.116 101.596 1.00 55.26	N
ATOM	6464 CA LYS D 401	35.988 24.084 100.747 1.00 55.15	С
ATOM	6465 C LYS D 401	35.619 24.315 99.276 1.00 54.36	С
ATOM	6466 O LYS D 401	34.456 24.152 98.883 1.00 53.30	0
		36.607 22.703 100.773 1.00 57.46	С
ATOM	6468 CG LYS D 401	36.857 22.055 102.095 1.00 60.83	С
ATOM	6469 CD LYS D 401	38.357 21.996 102.346 1.00 64.64	С
ATOM	6470 CE LYS D 401		С
ATOM	6471 NZ LYS D 401	37.772 20.479 104.196 1.00 70.44	N
ATOM	6472 N LEUD 402	36.677 24.687 98.529 1.00 51.63	N
ATOM	6473 CA LEU D 402	36.481 24.885 97.108 1.00 49.28	С
	6474 C LEU D 402	37.432 23.955 96.365 1.00 48.72	С
		38.646 24.038 96.510 1.00 49.51	0
		36.691 26.311 96.652 1.00 48.95	C
		35.857 27.437 97.251 1.00 48.74	C
		36.524 28.796 97.010 1.00 48.73	C
		34.438 27.390 96.713 1.00 47.64	C
	6480 N LEU D 403	36.886 23.079 95.559 1.00 47.56	N
	6481 CA LEU D 403	37.661 22.157 94.763 1.00 47.51	C C
	6482 C LEUD 403	38.046 22.737 93.418 1.00 47.68	0
ATOM		37.391 22.436 92.405 1.00 48.52	C
ATOM		36.733 20.948 94.527 1.00 48.78	C
		37.468 19.675 94.109 1.00 49.22 37.960 18.999 95.365 1.00 49.67	C
		36.624 18.756 93.259 1.00 48.96	C
		39.100 23.533 93.300 1.00 46.77	N
ATOM	6489 CA PHE D 404	39.468 24.057 91.990 1.00 46.77	C
ATOM		39.733 22.892 91.068 1.00 47.69	c
	6491 O PHE D 404		Ö
	6492 CB PHE D 404	40.670 24.998 92.034 1.00 45.47	C
	6493 CG PHE D 404	40.214 26.288 92.661 1.00 45.16	C
	6494 CD1 PHE D 404	40.200 26.430 94.033 1.00 44.79	С
	6495 CD2 PHE D 404	39.788 27.331 91.850 1.00 45.19	C .
	6496 CE1 PHE D 404	39.754 27.624 94.587 1.00 45.59	С
	6497 CE2 PHE D 404	39.349 28.521 92.385 1.00 44.20	С
ATOM	6498 CZ PHE D 404	39.339 28.659 93.752 1.00 45.30	С
ATOM	6499 N ALA D 405	40.410 21.876 91.548 1.00 50.13	N
	6500 CA ALA D 405	40.730 20.666 90.804 1.00 52.20	С
	6501 C ALA D 405	40.531 19.461 91.705 1.00 53.17	C
	6502 O ALA D 405	40.430 19.522 92.927 1.00 54.84	0
	6503 CB ALA D 405	42.170 20.689 90.327 1.00 51.92	Ç
		40.555 18.288 91.120 1.00 53.68	N
ATOM	6505 CA PRO D 406	40.455 17.023 91.830 1.00 53.61	С

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АТОМ	6506 C PRO D 406	41.649 17.004 92.777 1.00 54.39	С
ATOM	6507 O PRO D 406	41.444 16.490 93.860 1.00 56.81	Ō
		40.521 15.891 90.808 1.00 53.28	С
		40.346 16.616 89.511 1.00 53.32	
ATOM	6510 CD PRO D 406	40.743 18.070 89.684 1.00 54.19	
		42.801 17.531 92.398 1.00 53.35	N
		43.951 17.577 93.236 1.00 53.92	C
	6513 C ASN D 407		C
		45.461 19.263 94.028 1.00 58.16	O C
		45.079 17.006 92.383 1.00 54.30 45.564 17.970 91.342 1.00 54.63	C
		44.772 18.617 90.708 1.00 54.53	
ATOM	6518 ND2 ASN D 407	46.870 18.077 91.169 1.00 57.13	N
	6519 N LEUD 408		N
		43.601 21.230 94.408 1.00 54.93	C
		42.307 21.584 95.138 1.00 55.30	С
		41.306 21.854 94.501 1.00 54.97	0
		43.968 22.297 93.414 1.00 54.10	С
		44.225 23.714 93.898 1.00 54.18	С
ATOM	6525 CD1 LEU D 408	45.153 23.760 95.105 1.00 53.84	С
		44.807 24.546 92.745 1.00 53.64	С
		42.355 21.478 96.464 1.00 56.22	N
		41.152 21.729 97.268 1.00 55.14	С
		41.443 22.770 98.317 1.00 55.47	C
		41.823 22.462 99.442 1.00 57.57 40.769 20.366 97.801 1.00 54.10	O C
		39.635 20.138 98.762 1.00 54.26	C
		38.452 21.061 98.608 1.00 54.23	
		39.118 18.710 98.542 1.00 55.33	Č
		41.323 24.045 97.996 1.00 55.80	N
	6536 CA LEU D 410	41.596 25.095 98.963 1.00 56.04	С
ATOM	6537 C LEUD 410	40.411 25.166 99.914 1.00 58.15	С
		39.280 24.761 99.660 1.00 58.07	0
		41.934 26.433 98.332 1.00 54.82	C
		42.930 26.274 97.165 1.00 53.89	C
		43.178 27.583 96.458 1.00 54.38	С
		44.208 25.711 97.735 1.00 54.32	C
	6543 N ASP D 411	40.775 25.690 101.066 1.00 60.57 39.873 25.851 102.194 1.00 63.28	N C
	6544 CA ASP D 411 6545 C ASP D 411	39.639 27.330 102.396 1.00 63.04	c
		40.497 28.143 102.070 1.00 62.61	0
		40.604 25.118 103.304 1.00 67.29	C
		40.349 25.738 104.655 1.00 71.89	Č
		40.851 26.870 104.877 1.00 73.52	0
		39.629 25.053 105.439 1.00 74.78	0
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4 TO 1 4	6506 CD CVCD 417	47 262 32 815 100 634 1 00 68 39	С
ATOM	6507 SG CVS D 417	47.262 32.815 100.634 1.00 68.39 47.427 31.592 101.951 1.00 73.49	Š
ATOM	6508 N VAI D 418	45.893 35.461 99.383 1.00 62.39	N
ATOM	6599 CA VALD 418	45.860 36.548 98.426 1.00 60.27	
		44.980 37.688 98.902 1.00 61.04	
ATOM	6601 O VAL D 418	43.903 37.466 99.445 1.00 60.87	O
ATOM	6602 CB VAL D 418	45.360 36.041 97.073 1.00 59.10	С
ATOM	6603 CG1 VAL D 418	45,183 37,173 96,080 1.00 58.79	С
ATOM	6604 CG2 VAL D 418	46.314 34.983 96.546 1.00 58.31	С
ATOM	6605 N GLU D 419	45.428 38.912 98.712 1.00 62.71	N
ATOM	6606 CA GLUD 419	44.716 40.116 99.093 1.00 65.35	С
ATOM	6607 C GLU D 419	43.332 40.190 98.494 1.00 64.60	C
ATOM	6608 O GLU D 419	43.065 39.945 97.322 1.00 65.26	0_
ATOM	6609 CB GLUD 419	45.537 41.284 98.568 1.00 70.24	C
ATOM	6610 CG GLUD 419	45.668 42.507 99.451 1.00 76.95	C
ATOM	6611 CD GLUD 419	46.113 43.758 98.685 1.00 81.24	С
ATOM	6612 OE1 GLU D 419	46.881 43.691 97.679 1.00 82.62 45.696 44.889 99.073 1.00 83.42	0
ATOM	6613 OE2 GLU D 419	45.696 44.889 99.073 1.00 83.42	O N
ATOM	6614 N GLY D 420	42.312 40.504 99.261 1.00 64.31	
ATOM	6615 CA GLY D 420	40.952 40.618 98.782 1.00 63.52 40.278 39.372 98.291 1.00 62.66	
		39.132 39.494 97.866 1.00 63.85	0
ATOM	6619 N MET D 421	40.830 38.189 98.353 1.00 61.96	
ATOM	6610 CA MET D 421	40.233 36.958 97.909 1.00 61.23	
ATOM	6620 C MET D 421	39.229 36.266 98.798 1.00 60.15	
		38.393 35.534 98.295 1.00 60.63	0
ATOM	6622 CB MET D 421	41.368 35.916 97.784 1.00 62.22	
ATOM	6623 CG MET D 421	41.916 35.960 96.369 1.00 63.61	С
ATOM	6624 SD MET D 421	41.148 34.624 95.448 1.00 63.00 42.379 33.382 95.900 1.00 65.22	S C
ATOM	6625 CE MET D 421	42.379 33.382 95.900 1.00 65.22	С
ATOM	6626 N VAL D 422	39.313 36.410 100.099 1.00 59.43	N
		38.441 35.785 101.056 1.00 58.24	С
ATOM	6628 C VAL D 422	36.983 36.109 100.795 1.00 57.82	C
		36.190 35.191 100.949 1.00 57.63	0
	6630 CB VAL D 422		С
	- - ·	38.766 35.009 103.410 1.00 59.06	C C
	6632 CG2 VAL D 422	39.881 37.096 102.667 1.00 60.18	N
	6633 N GLUD 423	36.646 37.343 100.455 1.00 58.12 35.263 37.713 100.211 1.00 58.27	C
	6634 CA GLUD 423	34.765 36.994 98.968 1.00 55.62	c
	6635 C GLU D 423 6636 O GLU D 423	33.628 36.547 98.970 1.00 56.46	Ö
	6637 CB GLU D 423	35.048 39.198 99.981 1.00 63.42	c
		35.607 40.072 101.091 1.00 69.69	C
	6639 CD GLU D 423		Č
		37.960 39.580 101.067 1.00 74.80	Ō
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ATOM 6677 N LEUD 428

ATOM 6678 CA LEU D 428

ATOM 6679 C LEU D 428 ATOM 6680 O LEUD 428

ATOM 6681 CB LEUD 428

ATOM 6682 CG LEU D 428

ATOM 6683 CD1 LEU D 428

ATOM 6684 CD2 LEU D 428

ATOM 6685 N LEU D 429

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N

31.633 32.531 96.925 1.00 42.70

31.151 30.140 97.192 1.00 41.91

30.313 29.314 96.779 1.00 42.48

33.070 30.931 95.734 1.00 39.31 33.510 31.798 94.557 1.00 38.32

35.002 31.635 94.331 1.00 38.19

32.761 31.369 93.301 1.00 39.42

31.572 30.144 98.456 1.00 41.27

31.688 31.231 96.268 1.00 41.62

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ATOM	6686 CA LEUD 429	31.106 29.081 99.350 1.00 40.57	С
		29.624 29.149 99.574 1.00 40.99	c
		28.927 28.132 99.528 1.00 42.18	0
ATOM	6689 CB LEU D 429	31.940 29.105 100.603 1.00 40.44	
ATOM	6690 CG LEUD 429	33.393 28.673 100.380 1.00 39.94	С
ATOM	6691 CD1 LEU D 429	34.220 29.148 101.544 1.00 41.13	С
ATOM	6692 CD2 LEU D 429	33.455 27.174 100.190 1.00 39.25	С
		29.084 30.334 99.778 1.00 40.85	
ATOM	6694 CA ALAD 430	27.658 30.515 99.970 1.00 40.65	C
ATOM	6695 C ALA D 430	26.865 30.012 98.778 1.00 42.44	C
		25.754 29.491 98.938 1.00 45.02 27.394 32.002 100.090 1.00 40.90	
ATOM	6698 N THR D 431	27.339 30.174 97.548 1.00 41.99	N
ATOM	6699 CA THR D 431	26.562 29.674 96.429 1.00 41.67	c
ATOM	6700 C THR D 431	26.562 29.674 96.429 1.00 41.67 26.632 28.170 96.457 1.00 42.17	c
ATOM	6701 O THR D 431	25.698 27.427 96.233 1.00 42.18	
ATOM	6702 CB THR D 431	27.210 30.134 95 114 1 00 42.80	C
ATOM	6703 OG1 THR D 431	27.425 31.538 95.287 1.00 43.83 26.328 29.798 93.924 1.00 42.25	Ο
ATOM	6704 CG2 THR D 431	26.328 29.798 93.924 1.00 42.25	С
		27.845 27.694 96.722 1.00 43.94	
ATOM	6706 CA SER D 432	28.113 26.258 96.733 1.00 45.18	C
ATOM	6707 C SER D 432	27.161 25.571 97.694 1.00 45.21 26.566 24.533 97.490 1.00 44.06	C
ATOM	6700 CD SER D 432	29.597 26.004 97.039 1.00 44.71	0
		29.733 24.588 96.992 1.00 46.22	
		27.009 26.186 98.839 1.00 46.87	
ATOM	6712 CA SER D 433	26.148 25.773 99.910 1.00 49.54	C
		24.695 25.808 99.488 1.00 50.44	
ATOM	6714 O SER D 433	23.986 24.827 99.672 1.00 51.36	0
ATOM	6715 CB SER D 433	26.388 26.859 100.967 1.00 51.99 25.889 26.318 102.168 1.00 56.70	С
	6717 N ARG D 434	24.230 26.902 98.878 1.00 50.98	N
	6718 CA ARG D 434	22.866 26.983 98.398 1.00 51.45	C
	6719 C ARG D 434	22.667 25.859 97.401 1.00 51.71	C
	6720 O ARG D 434	21.629 25.218 97.447 1.00 51.99	O C
	6721 CB ARG D 434 6722 CG ARG D 434	22.500 28.356 97.835 1.00 52.96 21.112 28.377 97.229 1.00 55.73	C
	6723 CD ARG D 434	20.248 29.562 97.578 1.00 59.02	C
	6724 NE ARG D 434	18.818 29.386 97.162 1.00 61.34	N
	6725 CZ ARG D 434	18.049 28.559 97.888 1.00 62.31	Ċ
	6726 NH1 ARG D 434	18.586 27.916 98.937 1.00 63.44	N
	6727 NH2 ARG D 434	16.779 28.329 97.626 1.00 62.37	N
ATOM	6728 N PHE D 435	23.601 25.561 96.505 1.00 53.07	N
•	6729 CA PHE D 435	23.390 24.473 95.565 1.00 55.49	С
ATOM	6730 C PHE D 435	23.233 23.160 96.327 1.00 56.68	С

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ΔΤΟΜ	6776 C LEU D 440	21.482 19.488 91.649 1.00 59.80	С
		22.502 18.898 91.974 1.00 59.93	Ō
ATOM	6778 CB LEUD 440	21.877 21.934 92.171 1.00 57.04	C
ATOM	6779 CG LEUD 440	22.209 22.280 90.727 1.00 55.79	С
ATOM	6780 CD1 LEU D 440	20.992 22.898 90.077 1.00 55.60	С
		23.398 23.211 90.649 1.00 56.07	С
		20.729 19.111 90.627 1.00 60.60	N
ATOM	6783 CA GLN D 441	21.067 17.981 89.792 1.00 61.02	С
		22.036 18.348 88.699 1.00 59.67	С
ATOM	6785 O GLN D 441	22.047 19.490 88.298 1.00 60.79	0
ATOM	6786 CB GLN D 441	19.784 17.547 89.071 1.00 63.67	С
ATOM	6787 CG GLN D 441	18.746 16.948 89.995 1.00 67.17 19.375 16.015 91.025 1.00 69.21	С
ATOM	6788 CD GLN D 441	19.375 16.015 91.025 1.00 69.21	С
ATOM	6789 OE1 GLN D 441	19.706 14.899 90.611 1.00 70.52	0
ATOM	6790 NE2 GLN D 441	19.536 16.461 92.274 1.00 69.73	N
ATOM	6791 N GLY D 442	22.784 17.416 88.158 1.00 59.13	N
ATOM	6792 CA GLY D 442	23.713 17.697 87.078 1.00 56.87	С
ATOM	6793 C GLY D 442	22.979 18.101 85.824 1.00 56.45	С
ATOM	6794 O GLY D 442	23.546 18.922 85.108 1.00 56.38	0
		21.780 17.593 85.534 1.00 56.59	
		21,083 18.001 84.315 1.00 57.10	
ATOM	6797 C GLU D 443	20.719 19.479 84.468 1.00 54.01	C
ATOM	6798 O GLU D 443	20.759 20.200 83.499 1.00 53.31	0
ATOM	6799 CB GLU D 443	19.818 17.241 83.962 1.00 61.47	C
ATOM	6800 CG GLU D 443	19.787 15.730 83.877 1.00 64.56	C
ATOM	6801 CD GLU D 443	20.350 15.084 85.131 1.00 66.39	C
ATOM	6802 OE1 GLU D 443	20.020 15.514 86.252 1.00 67.30	
ATOM	6803 OE2 GLU D 443	21.152 14.148 84.960 1.00 67.90	0
		20.362 19.872 85.680 1.00 51.49	N
		20.031 21.253 85.994 1.00 48.76	C
	6806 C GLUD 444		C
ATOM	6807 O GLUD 444	21.284 23.084 85.088 1.00 48.04	O C
		19.563 21.350 87.437 1.00 48.48	C
ATOM	6809 CG GLU D 444	18.148 20.791 87.568 1.00 48.45	C
		17.672 20.825 89.007 1.00 48.07	O
ATOM	6811 OEI GLU D 444	18.484 20.503 89.894 1.00 46.60	0
		16.487 21.181 89.132 1.00 48.63 22.367 21.654 86.413 1.00 45.51	N
	6813 N PHE D 445	23.650 22.321 86.311 1.00 44.62	C
	6814 CA PHE D 445	23.980 22.706 84.875 1.00 44.77	c
	6815 C PHE D 445	24.234 23.841 84.512 1.00 45.62	O
	6816 O PHE D 445	24.794 21.461 86.864 1.00 43.02	C
			Č
		26.138 21.994 86.339 1.00 41.93	C
		27.057 21.271 85.831 1.00 41.88	C
AIUM	0020 CD2 FRE D 443	21,031 21.211 03.031 1.00 41.00	•

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ATO) (6001	CEL DUE D 445	27.795 23.757 86.729 1.00 42.63 28.325 21.740 85.532 1.00 41.96 28.683 22.990 85.987 1.00 43.00	C
ATOM	6822	CE1 PRE D 443	28 325 21 740 85 532 1 00 41 96	C
ATOM	6823	CZ PHE D 445	28.683 22.990 85.987 1.00 43.00	C
ATOM	6824	N VAL D 446	24.011 21.738 84.006 1.00 44 .75	N
ATOM	6825	CA VAL D 446	24.323 21.845 82.595 1.00 44.55	С
ATOM	6826	C VAL D 446	24.323 21.845 82.595 1.00 44.55 23.423 22.850 81.915 1.00 45.82	С
ATOM	6827	O VAL D 446	23.856 23.614 81.021 1.00 46.31	O
ATOM	6828	CB VAL D 446	24.348 20.374 82.130 1.00 43.66	С
ATOM	6829	CG1 VAL D 446	23.502 20.001 80.941 1.00 43.51 25.797 20.021 81.897 1.00 43.07	С
ATOM	6830	CG2 VAL D 446	25.797 20.021 81.897 1.00 43.07	С
ATOM	6831	N CYS D 447	22.153 22.923 82.294 1.00 46.23	N
ATOM	6832	CA CYS D 447	21.235 23.886 81.701 1.00 47.72	С
ATOM	6833	C CYS D 447	21.530 25.334 82.093 1.00 47.52 21.531 26.206 81.246 1.00 46.80 19.827 23.550 82.214 1.00 48.91	C
ATOM	6834	O CYS D 447	21.531 26.206 81.246 1.00 46.80	0
ATOM	6835	CB CYS D 447	19.827 23.550 82.214 1.00 48.91	C
ATOM	6836	SG CYS D 447	18.991 22.336 81.203 1.00 50.22	S
ATOM	6837	N LEU D 448	21.738 25.570 83.391 1.00 46.99	N
ATOM	6838	CA LEU D 448	21.738 25.570 83.391 1.00 46.99 22.070 26.868 83.934 1.00 45.68 23.332 27.419 83.290 1.00 44.95	C
ATOM	6839	C LEU D 448	23.332 27.419 83.290 1.00 44.93	0
ATOM	6840	CD LEUD 448	23.429 28.572 82.884 1.00 45.79 22.314 26.760 85.434 1.00 45.92	C
ATOM	6041	CG LEUD 448	21.003 26.655 86.347 1.00.45.80	C
ATOM	6843	CD1 I FII D 448	21.617 26.450 87.757 1.00 46.68	C
ATOM	6844	CD2 LEU D 448	21.093 26.655 86.347 1.00 45.80 21.617 26.450 87.757 1.00 46.68 20.193 27.878 86.304 1.00 44.62	Č
$\Delta T \Omega M$	6845	N LYS D 449	24 331 26 561 83 154 1.00 44.17	N
ATOM	6846	CA LYS D 449	25.599 26.948 82.536 1.00 43.37	С
ATOM	6847	C LYS D 449	25.599 26.948 82.536 1.00 43.37 25.338 27.458 81.139 1.00 42.62 25.877 28.518 80.806 1.00 43.03	С
ATOM	6848	O LYS D 449	25.877 28.518 80.806 1.00 43.03	0
$\lambda T \Omega \lambda I$	6840	CB I VC D 440	26 554 25 791 82 659 1 00 43 95	C
ATOM	6850	CG LYS D 449	28.009 26.153 82.807 1.00 44.50	С
ATOM	6851	CD LYS D 449	28.009 26.153 82.807 1.00 44.50 28.769 25.193 81.908 1.00 45.79	C
ATOM	6852	CE LYS D 449	29.224 23.981 82.706 1.00 46.49	C
			30.163 23.282 81.735 1.00 49.77	N
		N SER D 450		N
		CA SER D 450	24.238 27.374 78.992 1.00 41.89	C
		C SER D 450	23.410 28.642 79.057 1.00 40.65	C
		O SER D 450	23.605 29.481 78.202 1.00 41.51	O C
			23.432 26.431 78.101 1.00 42.84 24.173 25.209 78.223 1.00 46.38	0
		OG SER D 450 N ILE D 451	24.173 25.209 78.223 1.00 40.36	N
			21.698 29.976 80.148 1.00 37.93	C
		C ILE D 451		c
			22.518 32.116 79.704 1.00 37.47	Ö
			20.725 29.872 81.329 1.00 38.37	C
			19.741 28.776 80.952 1.00 38.67	С

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4 TO 3 (6966 CC2 TI E D 451	262/371 20.093 31.213 81.662 1.00 37.38	C
		18.514 28.737 81.822 1.00 41.51	
ATOM	6868 N ILE D 452	23.676 30.877 81.240 1.00 37.60	N
ATOM	6869 CA ILE D 452	24.691 31.886 81.525 1.00 36.56	С
ATOM	6870 C ILE D 452	25.436 32.257 80.256 1.00 36.13	С
ATOM	6871 O ILE D 452	25.610 33.434 80.030 1.00 36.37 25.730 31.436 82.579 1.00 35.77	O
ATOM	6872 CB ILE D 452	25.730 31.436 82.579 1.00 35.77	С
		25.014 31.155 83.900 1.00 34.24	
ATOM	6874 CG2 ILE D 452	26.844 32.461 82.723 1.00 34.78	C
ATOM	6875 CD1 ILE D 452	25.892 30.989 85.099 1.00 33.24	C
ATOM	68/6 N LEUD 453	25.838 31.286 79.452 1.00 36.42 26.549 31.553 78.228 1.00 36.94	N C
		25.696 32.400 77.310 1.00 38.42	
ATOM	6879 O LEUD 453	26.173 33.323 76.682 1.00 39.35	O
ATOM	6880 CB LEU D 453	26.968 30.277 77.478 1.00 35.54	C
ATOM	6881 CG LEU D 453	27.531 30.530 76.067 1.00 35.05	C
ATOM	6882 CD1 LEU D 453	28.844 31.294 76.058 1.00 33.75	
ATOM	6883 CD2 LEU D 453	27.718 29.250 75.299 1.00 34.02	С
ATOM	6884 N LEU D 454	24.431 32.083 77.160 1.00 41.14	N
		23.570 32.821 76.262 1.00 43.55	
		22.976 34.121 76.765 1.00 44.50	
ATOM	6887 O LEUD 454	22.805 35.002 75.913 1.00 46.40	0
ATOM	6888 CB LEU D 454	22.380 31.917 75.839 1.00 43.39	C
		22.823 30.835 74.849 1.00 43.72	
		21.789 29.750 74.787 1.00 44.06 23.000 31.428 73.468 1.00 44.69	
	6892 N ASN D 455		N
		21.990 35.492 78.456 1.00 45.22	
		22.911 36.573 78.923 1.00 48.85	
		22.447 37.720 78.958 1.00 51.01	0
		21.026 35.166 79.579 1.00 44.21	С
	6897 CG ASN D 455	20.481 36.271 80.419 1.00 43.95	С
	6898 OD1 ASN D 455	20.909 36.409 81.568 1.00 44.44	0
	6899 ND2 ASN D 455	19.557 37.057 79.888 1.00 43.94	N
	6900 N SER D 456	24.141 36.290 79.297 1.00 52.15	N
	6901 CA SER D 456	24.949 37.375 79.841 1.00 55.13	C
	6902 C SER D 456 6903 O SER D 456	25.284 38.474 78.866 1.00 57.33 25.192 39.676 79.158 1.00 58.90	C O
	6904 CB SER D 456	26.177 36.767 80.523 1.00 55.03	C
	6905 OG SER D 456	25.851 36.397 81.835 1.00 53.67	Ö
	6906 N GLY D 457	25.695 38.152 77.664 1.00 59.87	N
	6907 CA GLY D 457	26.071 39.211 76.728 1.00 63.73	C
	6908 C GLY D 457	24.984 39.616 75.764 1.00 65.27	C
	6909 O GLY D 457	25.290 40.349 74.835 1.00.64.43	0
ATOM	6910 N VAL D 458	23.767 39.137 75.986 1.00 68.09	N

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		22.681 39.469 75.080 1.00 71.03	С
		22.321 40.933 74.994 1.00 74.49	C
		22.036 41.364 73.869 1.00 75.49	0
		21.475 38.547 75.320 1.00 69.39	С
		20.688 38.875 76.549 1.00 68.27	С
ATOM	6916 CG2 VAL D 458	20.585 38.594 74.081 1.00 69.67	С
ATOM	6917 N TYR D 459	22.356 41.782 75.995 1.00 78.79	N
ATOM	6918 CA TYR D 459	22.008 43.181 75.933 1.00 83.41	С
ATOM	6919 C TYR D 459	23.164 44.036 75.477 1.00 85.77	С
ATOM	6920 O TYR D 459	23.175 45.241 75.717 1.00 87.22	Ο
ATOM	6921 CB TYR D 459	21.561 43.737 77.319 1.00 85.69	С
ATOM	6922 CG TYR D 459	20.493 42.800 77.854 1.00 87.98	С
		20.862 41.683 78.595 1.00 88.70	С
ATOM	6924 CD2 TYR D 459	19.147 43.003 77.594 1.00 88.99	С
		19.896 40.820 79.060 1.00 90.23	C
ATOM	6926 CE2 TYR D 459	18.177 42.130 78.049 1.00 90.00	С
		18.552 41.030 78.792 1.00 90.79	C
		17.609 40.133 79.271 1.00 91.09	Ο
		24.163 43.468 74.843 1.00 88.54	N
		25.327 44.222 74.394 1.00 90.99	С
		25.819 43.676 73.061 1.00 92.45	C
		27.027 43.515 72.869 1.00 93.66	0
		26.450 44.148 75.445 1.00 91.16	С
ATOM	6934 OG1 THR D 460	26.154 43.307 76.561 1.00 91.27	О
ATOM	6935 CG2 THR D 460	26.656 45.535 76.037 1.00 92.12	С
	6936 N PHE D 461		N
		25.314 42.844 70.878 1.00 94.98	С
ATOM	6938 C PHE D 461		C
ATOM		27.113 43.214 69.399 1.00 97.69	0
ATOM		24.119 42.166 70.170 1.00 94.65	C
ATOM	6941 CG PHE D 461	24.263 40.679 70.430 1.00 93.76	C
		25.524 40.13770.616 1.00 93.43	·C
ATOM	6943 CD2 PHE D 461	23.176 39.849 70.503 1.00 93.49	C
ATOM		25.726 38.809 70.870 1.00 93.10	C
	6945 CE2 PHE D 461	23.368 38.511 70.750 1.00 93.62	C
	6946 CZ PHE D 461	24.631 37.983 70.932 1.00 93.40	C
ATOM	6947 N THR D 465	22.624 45.967 63.550 1.00127.65	N
ATOM	6948 CA THR D 465	21.376 46.227 64.267 1.00127.69	С
ATOM	6949 C THR D 465	20.289 45.238 63.883 1.00126.64	С
ATOM	6950 O THR D 465	19.950 44.353 64.675 1.00127.34	·O
ATOM	6951 CB THR D 465	20.851 47.661 64.084 1.00128.43	C
ATOM		19.424 47.705 64.272 1.00128.82	0
	6953 CG2 THR D 465	21.170 48.197 62.693 1.00128.79	С
ATOM	6954 N LEUD 466	19.741 45.302 62.672 1.00124.51	N
ATOM	6955 CA LEU D 466	18.705 44.356 62.251 1.00122.04	С

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4 TO 14	6056 C TELLD 466	264/371	С
	6956 C LEUD 466 6957 O LEUD 466	19.174 42.908 62.392 1.00119.80 18.380 42.001 62.689 1.00119.83	0
	6958 CB LEU D 466	18.239 44.686 60.837 1.00122.41	C
	6962 N LYS D 467	20.472 42.656 62.200 1.00116.36	N
		21.041 41.328 62.370 1.00112.85	
	6964 C LYS D 467	21.062 41.103 63.887 1.00108.83	С
ATOM	6965 O LYS D 467	20.845 39.985 64.333 1.00108.82	0
		22.439 41.155 61.790 1.00114.37	С
		22.851 39.725 61.452 1.00115.62	С
		24.347 39.658 61.199 1.00117.19	C
		24.756 39.606 59.729 1.00117.88	
		26.238 39.769 59.560 1.00117.63	
	6971 N SER D 468		N C
	6972 CA SER D 468 6973 C SER D 468	21.303 42.054 66.114 1.00 99.58 19.922 41.722 66.669 1.00 96.01	C
		19.782 40.953 67.608 1.00 95.40	0
		21.709 43.362 66.797 1.00100.34	C
		23.064 43.653 66.528 1.00101.77	Ö
		18.903 42.320 66.067 1.00 92.13	N
		17.527 42.083 66.486 1.00 88.58	С
ATOM	6979 C LEUD 469	17.207 40.624 66.216 1.00 86.29	С
		16.507 39.969 66.976 1.00 85.00	Ο
		16.606 43.082 65.801 1.00 89.09	С
			N
		17.526 38.684 64.759 1.00 83.02	С
	6987 C GLUD 470		С
		17.939 36.776 66.149 1.00 77.81	0
		17.772 38.529 63.280 1.00 87.02 18.612 37.362 62.816 1.00 92.72	C C
ATOM	6990 CO GLUD 470	19.073 37.527 61.375 1.00 96.70	C
	6992 OE1 GLU D 470	18.960 38.661 60.822 1.00 98.66	Ö
	6993 OE2 GLU D 470	19.551 36.519 60.786 1.00 98.72	Ö
	6994 N GLUD 471	19.596 38.228 65.989 1.00 75.15	N
	6995 CA GLUD 471	20.506 37.543 66.889 1.00 70.77	С
ATOM	6996 C GLU D 471	19.871 37.513 68.283 1.00 69.37	С
ATOM	6997 O GLU D 471	19.873 36.498 68.972 1.00 68.92	0
	6998 CB GLU D 471	21.863 38.216 66.977 1.00 69.02	С
	6999 CG GLU D 471	22.727 38.202 65.767 1.00 67.63	C
		23.780 37.140 65.725 1.00 68.27	С
ATOM		24.767 37.192 66.463 1.00 67.40	0
ATOM	7002 OE2 GLU D 471	23.681 36.173 64.932 1.00 69.91	O N
ATOM	7003 N LYS D 472 7004 CA LYS D 472	19.311 38.636 68.724 1.00 68.00	N C
ATOM ATOM	7004 CA LYSD 472 7005 C LYSD 472	18.643 38.704 70.011 1.00 66.62 17.455 37.755 70.031 1.00 64.90	C
ATOM	7006 O LYS D 472	17.316 37.050 71.014 1.00 65.02	Ö
		1 51.050 11.011 1.00 00.02	-

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ATOM	7007 CB LYS D 472	18.168 40.104 70.395 1.00 67.81	С
		19.292 41.038 70.752 1.00 70.56	Č
ATOM	7009 CD LYS D 472	18.827 42.323 71.380 1.00 73.00	Č
ATOM	7010 CE LYS D 472	19.691 43.522 71.019 1.00 75.44	С
ATOM	7011 NZ LYS D 472	20.894 43.754 71.896 1.00 77.11	N
		16.602 37.676 69.030 1.00 64.19	N
ATOM	7013 CA ASP D 473	15.466 36.783 69.058 1.00 64.15	
ATOM	7014 C ASP D 473	15.899 35.335 69.128 1.00 61.42	C
ATOM	7015 O ASP D 473	15.385 34.559 69.902 1.00 62.62	0
ATOM	7016 CB ASP D 473	14.611 36.829 67.796 1.00 68.83	C
ATOM	7017 CG ASP D 473	13.999 38.198 67.618 1.00 73.25	С
ATOM	7018 OD1 ASP D 473	14.079 39.069 68.518 1.00 75.35	0 0
ATOM	7019 ODZ ASP D 473	13.409 38.384 66.527 1.00 76.20 16.838 34.967 68.286 1.00 57.77	N
ATOM	7020 N HIS D 474	17.345 33.610 68.285 1.00 54.52	C
ATOM	7021 CA M3 D 474	17.726 33.238 69.714 1.00 53.80	c
ATOM	7022 C IIIS D 474	17.292 32.240 70.293 1.00 52.80	Ö
		18.570 33.612 67.358 1.00 53.69	Č
		19.062 32.195 67.328 1.00 53.28	Č
ATOM	7026 ND1 HIS D 474	18.207 31.170 66.988 1.00 52.17	
ATOM	7027 CD2 HIS D 474	20.267 31.676 67.651 1.00 53.88	С
ATOM	7028 CE1 HIS D 474	20.267 31.676 67.651 1.00 53.88 18.892 30.051 67.065 1.00 53.66	С
ATOM	7029 NE2 HIS D 474	20.131 30.321 67.468 1.00 54.49	N
ATOM	7030 N ILE D 475	18.586 34.047 70.342 1.00 53.00	
		19.002 33.822 71.705 1.00 52.51	C
ATOM	7032 C ILE D 475	17.794 33.715 72.609 1.00 52.34	C
ATOM	7033 O ILE D 475	17.680 32.717 73.325 1.00 51.65	0
ATOM	7034 CB ILE D 475	19.957, 34.910, 72.201, 1.00, 53.42	C C
ATOM	7035 CG1 ILE D 475	21.273 34.733 71.434 1.00 53.48	C
ATOM	7037 CD1 ILE D 475	20.174 34.816 73.709 1.00 53.71 22.329 35.716 71.891 1.00 53.61	C
VIOIN	7038 N HIS D 476	16.885 34.674 72.601 1.00 53.82	N
ATOM	7039 CA HIS D 476	15.700 34.570 73.454 1.00 56.40	C
	7040 C HIS D 476	14.964 33.260 73.213 1.00 57.06	c
	7041 O HIS D 476	14.536 32.605 74.163 1.00 57.87	0
ATOM		14.776 35.765 73.299 1.00 58.36	С
ATOM	7043 CG HIS D 476	15.381 36.987 73.932 1.00 59.96	С
ATOM	7044 ND1 HIS D 476	15.964 36.937 75.168 1.00 60.20	N .
	7045 CD2 HIS D 476	15.490 38.263 73.490 1.00 60.94	C
	7046 CE1 HIS D 476		C
		16.146 38.983 74.461 1.00 60.99	N
	7048 N ARG D 477		N
	7049 CA ARG D 477	14.197 31.586 71.587 1.00 57.91	C
ATOM		14.841 30.342 72.177 1.00 56.02 14.134 29.464 72.665 1.00 56.11	C O
ATOM	7051 O ARG D 477	14.134 29.404 /2.003 1.00 30.11	U

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ATOM	7052 CB ARG D 477	14.316 31.406 70.069 1.00 62.44	C C
ATOM	7053 CG ARG D 4//	13.037 30.852 69.468 1.00 67.89	C
ATOM	7054 CD ARG D 4//	12.106 32.067 69.294 1.00 73.64 12.755 32.943 68.307 1.00 79.62	C N
		12.755 32.943 68.307 1.00 79.02	N C
ATOM		12.723 32.654 66.993 1.00 82.77	
ATOM	7057 NH1 ARG D 477	12.074 31.552 66.581 1.00 84.58	
ATOM	7058 NH2 ARG D 477	13.327 33.463 66.125 1.00 83.31	N
ATOM	7059 N VAL D 478	16.164 30.245 72.108 1.00 53.51	N
ATOM	7060 CA VAL D 478	16.899 29.103 72.662 1.00 50.86	C
ATOM	7061 C VAL D 478	16.752 29.150 74.171 1.00 49.96	C
ATOM	7062 O VAL D 478	16.558 28.175 74.891 1.00 50.09	0
ATOM	7063 CB VAL D 478	18.382 29.178 72.250 1.00 50.20	C
ATOM	7064 CG1 VAL D 478	19.216 28.029 72.758 1.00 48.27	C
		18.446 29.262 70.725 1.00 50.29	C
		16.795 30.363 74.733 1.00 48.62	N
		16.616 30.525 76.169 1.00 47.30	С
ATOM	7068 C LEU D 479	15.276 29.961 76.605 1.00 48.58	C
ATOM	7069 O LEU D 479	15.220 29.398 77.701 1.00 49.89	0
ATOM	7070 CB LEU D 479	16.775 31.980 76.570 1.00 44.30	C
		18.221 32.407 76.806 1.00 41.99	
		18.316 33.919 76.921 1.00 41.99	C C
		18.795 31.728 78.021 1.00 40.35	
		14.210 30.084 75.818 1.00 49.32	N C
		12.914 29.543 76.184 1.00 48.95	c
		12.997 28.035 76.109 1.00 49.02	0
ATOM	7077 O ASP D 480	12.503 27.345 76.972 1.00 48.57	C
ATOM	7078 CB ASP D 480	11.818 30.030 75.284 1.00 50.60 11.434 31.479 75.430 1.00 52.07	C
ATOM	7079 CG ASP D 480	11.434 31.479 73.430 1.00 32.07	
		11.626 32.083 76.497 1.00 52.84 10.914 32.052 74.437 1.00 53.13	Ö
		13.653 27.514 75.096 1.00 51.64	N
	7083 CA LYS D 481	13.813 26.069 74.922 1.00 53.47	C
		14.538 25.531 76.137 1.00 52.34	c
	7085 O LYS D 481	14.057 24.571 76.712 1.00 53.37	Ö
	7086 CB LYS D 481	14.582 25.684 73.664 1.00 56.66	Č
	7087 CG LYS D 481	14.441 24.208 73.351 1.00 61.56	Č
	7088 CD LYS D 481	13.285 23.957 72.380 1.00 65.28	Č
	7089 CE LYS D 481	12.750 22.535 72.454 1.00 67.98	č
	7090 NZ LYS D 481	12.998 21.867 73.776 1.00 70.18	N
	7091 N ILE D 482	15.627 26.170 76.564 1.00 50.96	N
	7092 CA ILE D 482	16.337 25.699 77.749 1.00 49.43	C
	7093 C ILE D 482	15.423 25.802 78.951 1.00 48.89	c
	7094 O ILE D 482	15.434 24.924 79.824 1.00 49.34	Ö
	7095 CB ILE D 482	17.681 26.367 77.979 1.00 49.26	C
		18.611 26.001 76.815 1.00 49.57	C
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ΔΤΟΜ	7097	CG2 ILE D 482	18.331 25.915 79.270 1.00 48.99	С
ATOM	7098	CD1 ILE D 482	19.441 27.195 76.405 1.00 49.58	С
ATOM	7099	N THR D 483	14.572 26.816 79.034 1.00 48.55	N
ATOM	7100	CA THR D 483	13.648 26.883 80.168 1.00 48.75	С
ATOM		C THR D 483	12.727 25.666 80.165 1.00 49.97	С
ATOM	7102	O THR D 483	12.480 25.027 81.188 1.00 50.53	0
ATOM	7103	CB THR D 483	12.796 28.149 80.107 1.00 47.82	С
ATOM	7104	OG1 THR D 483	13.740 29.204 80.281 1.00 48.13	O
ATOM	7105	CG2 THR D 483	11.734 28.119 81.182 1.00 47.64	С
ATOM	7106	N ASP D 484	12.221 25.336 78.964 1.00 49.96	N
ATOM	7107	CA ASP D 484	11.329 24.201 78.824 1.00 48.69	С
ATOM	7108	C ASP D 484	12.055 22.962 79.277 1.00 48.48	C
ATOM	7109	O ASP D 484	11.484 22.156 80.010 1.00 50.20	0
ATOM	7110	CB ASP D 484	10.818 24.054 77.419 1.00 49.22	C C
ATOM	7111	CG ASP D 484	9.855 25.145 77.025 1.00 50.77	0
ATOM	7112	OD1 ASP D 484	9.301 25.870 77.886 1.00 50.61 9.653 25.271 75.789 1.00 52.45	0
ATOM	7113	VDZ ASP D 484	13.310 22.799 78.886 1.00 47.73	N
ATOM	7114	CA THE D 485	14.055 21.610 79.302 1.00 47.73	
ATOM	7115	CA THE D 485	14.152 21.504 80.810 1.00 48.41	
ATOM	7117	O THR D 485	14.057 20.420 81.374 1.00 48.46	Ö
ATOM	7118	CB THR D 485	15.460 21.727 78.713 1.00 45.73	C
ATOM	7110	OG1 THR D 485	15.224 21.938 77.324 1.00 45.98	0
ATOM	7120	CG2 THR D 485	16.242 20.496 79.033 1.00 45.10	C
ATOM	7121	N LEUD 486	14.336 22.652 81.464 1.00 48.84	N
ATOM	7122	CA LEU D 486	14.445 22.680 82.908 1.00 49.26	С
ATOM	7123	C LEU D 486	13.173 22.222 83.594 1.00 50.81	С
ATOM	7124	O LEU D 486	13.225 21.422 84.521 1.00 50.74	0
ATOM	7125	CB LEUD 486	14.766 24.095 83.387 1.00 47.63	С
ATOM	7126	CG LEU D 486	16.242 24.335 83.695 1.00 46.21	C
			16.377 25.792 84.101 1.00 46.08	C
		CD2 LEU D 486	16.818 23.376 84.714 1.00 43.41	C
ATOM		N ILE D 487	12.031 22.742 83.137 1.00 52.73	N
ATOM		CA ILE D 487	10.736 22.360 83.707 1.00 53.30	C
ATOM		C ILE D 487	10.511 20.882 83.456 1.00 54.63	C
		O ILE D 487	10.065 20.157 84.323 1.00 54.41	O C
ATOM		CB ILE D 487	9.598 23.141 83.053 1.00 52.55 9.676 24.593 83.491 1.00 53.86	C
ATOM		CG1 ILE D 487 CG2 ILE D 487	8.283 22.509 83.415 1.00 53.12	Č
ATOM		CD1 ILE D 487	9.134 24.958 84.855 1.00 52.98	Č
ATOM ATOM		N HIS D 488	10.857 20.468 82.238 1.00 57.04	N
ATOM		CA HIS D 488	10.720 19.085 81.829 1.00 59.25	Ċ
ATOM		C HIS D 488	11.406 18.179 82.838 1.00 58.05	C
		O HIS D 488	10.892 17.222 83.368 1.00 57.71	0
			11.346 18.872 80.448 1.00 62.29	С
		 		

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ΔΤΟΜ	7142 CG HIS D 488	11.405 17.399 80.140 1.00 65.17	С
ATOM	7143 ND1 HIS D 488	10.283 16.647 79.880 1.00 66.20	N
ATOM	7144 CD2 HIS D 488	12.478 16.572 80.079 1.00 66.45	С
ATOM	7145 CE1 HIS D 488	12.478 16.572 80.079 1.00 66.45 10.692 15.405 79.660 1.00 67.99	С
ATOM	7146 NE2 HIS D 488	12.020 15.318 79.775 1.00 67.51	N
ATOM	7147 N LEUD 489	12.657 18.487 83.108 1.00 57.87	N
ATOM	7148 CA LEUD 489	13.449 17.742 84.055 1.00 57.53	С
ATOM	7149 C LEUD 489	12.778 17.642 85.404 1.00 58.23	
ATOM	7150 O LEUD 489	12.730 16.581 85.998 1.00 59.34	0
ATOM	7151 CB LEU D 489	14.777 18.483 84.230 1.00 57.04	C
ATOM	7152 CG LEUD 489	15.786 18.189 83.137 1.00 57.56	C
ATOM	7153 CD1 LEU D 489	16.973 19.125 83.290 1.00 58.88	C
ATOM	7154 CD2 LEU D 489	16.267 16.752 83.176 1.00 57.38	C
ATOM	7155 N MET D 490	12.284 18.722 85.953 1.00 59.22	N
ATOM	7156 CA MET D 490	11.641 18.827 87.233 1.00 59.67	· C
ATOM	7157 C MET D 490	10.329 18.068 87.318 1.00 60.84	С
ATOM	7158 O MET D 490	10.051 17.498 88.371 1.00 61.71	O C
ATOM	7159 CB MET D 490	11.319 20.304 87.492 1.00 59.79	
ATOM	7160 CG MEI D 490	12.404 21.038 88.234 1.00 59.24 12.190 22.803 88.134 1.00 57.81	S
ATOM	7161 SD MEI D 490	13.863 23.335 87.948 1.00 59.41	C
ATOM	7162 CE MEI D 490	9.549 18.101 86.237 1.00 61.24	=
ATOM	7164 CA AI A D 491	8 278 17 372 86 247 1 00 61.75	C
ATOM	7165 C. ALA D 491	8.278 17.372 86.247 1.00 61.75 8.674 15.904 86.334 1.00 61.95	C
ATOM	7166 O ALA D 491	8.204 15.123 87.136 1.00 61.50	0
ATOM	7167 CB ALA D 491	7.429 17.679 85.044 1.00 61.70	С
ATOM	7168 N LYS D 492	9.646 15.491 85.537 1.00 63.32	N
ATOM	7169 CA LYS D 492	10.146 14.128 85.511 1.00 64.48	С
ATOM	7170 C LYS D 492	10.578 13.747 86.903 1.00 65.18	С
ATOM	7171 O LYS D 492	10.428 12.584 87.273 1.00 67.28	
		11.221 13.848 84.463 1.00 63.79	С
	7177 N ALA D 493	11.041 14.629 87.765 1.00 66.09	N
	7178 CA ALAD 493	11.389 14.273 89.140 1.00 66.81	С
	7179 C ALA D 493	10.128 14.356 90.001 1.00 67.36	C
	7180 O ALA D 493	10.063 14.195 91.207 1.00 67.78	O C
	7181 CB ALA D 493	12.473 15.145 89.721 1.00 65.96 9.005 14.625 89.380 1.00 68.06	N
	7182 N GLY D 494	7.740 14.708 90.043 1.00 69.81	C
	7183 CA GLY D 494 7184 C GLY D 494	7.663 15.827 91.061 1.00 69.63	c
	7185 O GLY D 494	7.480 15.557 92.250 1.00 71.09	Ö
ATOM		7.765 17.081 90.656 1.00 68.58	N
ATOM		7.591 18.133 91.647 1.00 67.21	C
	7188 C LEU D 495	6.226 18.693 91.258 1.00 67.00	C
	7189 O LEU D 495	5.965 18.674 90.055 1.00 67.42	0
ATOM		8.577 19.265 91.570 1.00 67.41	С

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ATOM	7191	CG LEUD 495	10.064 19.001 91.516 1.00 67.23	С
			10.835 20.279 91.744 1.00 66.57	С
			10.474 17.996 92.580 1.00 68.59	С
ATOM	7194	N THR D 496	5.459 19.174 92.194 1.00 67.01	N
			4.175 19.743 91.803 1.00 68.57	С
ΔΤΟΜ	7196	C THR D 496	4 381 20 804 90 758 1 00 68.94	C
ATOM	7197	O THR D 496	5.466 21.344 90.612 1.00 70.43	Ο
ATOM	7198	CB THR D 496	5.466 21.344 90.612 1.00 70.43 3.642 20.474 93.043 1.00 69.67	С
ATOM	7199	OG1 THR D 496	3.559 19.460 94.038 1.00 70.00	O
ATOM	7200	CG2 THR D 496	2.303 21.162 92.843 1.00 72.03	С
ATOM	7201	N LEU D 497	3.354 21.242 90.073 1.00 69.68	N
ATOM	7202	CA LEUD 497	3.459 22.327 89.113 1.00 70.36	C
			3.924 23.570 89.853 1.00 70.71	C
ATOM	7204	O LEU D 497	4.636 24.418 89.326 1.00 71.29	0
ATOM	7205	CB LEU D 497	2.089 22.554 88.518 1.00 71.76	C
	7206	CG LEUD 497	1.898 22.725 87.025 1.00 72.92	C C
			1.027 23.981 86.893 1.00 74.10	
			3.226 22.851 86.288 1.00 73.59 3.526 23.722 91.110 1.00 71.33	N
		N GLN D 498 CA GLN D 498		C
		CA GLN D 498		c
			6.065 25.726 92.369 1.00 70.91	Ö
			3.011 25.127 93.108 1.00 74.58	
ATOM	7213	CG GLN D 498	3.668 25.956 94.183 1.00 77.41	-
			2.776 26.383 95.317 1.00 79.69	Ċ
			2.814 27.551 95.725 1.00 81.49	Ο
			1.968 25.482 95.863 1.00 80.48	N
		N GLN D 499		
	7219	CA GLN D 499	7.205 23.418 93.118 1.00 66.67	C
ATOM	7220	C GLN D 499	8.082 23.649 91.889 1.00 65.31	С
ATOM			9.207 24.131 91.996 1.00 66.02	. O
		CB GLN D 499	7.498 22.012 93.605 1.00 67.59	C
		CG GLN D 499	6.331 21.445 94.385 1.00 68.83	C
		CD GLN D 499	6.815 20.277 95.218 1.00 69.76	C
		OE1 GLN D 499	7.094 19.197 94.705 1.00 71.19	0.
		NE2 GLN D 499	6.905 20.540 96.506 1.00 69.95	N
		N GLN D 500	7.564 23.270 90.726 1.00 62.76	N
		CA GLN D 500	8.296 23.482 89.499 1.00 61.09	C C
_		C GLN D 500	8.517 24.994 89.331 1.00 59.09 9.691 25.383 89.229 1.00 59.14	0
		O GLN D 500	7.540 22.919 88.315 1.00 62.27	C
		CB GLN D 500 CG GLN D 500	7.714 21.442 88.024 1.00 62.80	C
_		CD GLN D 500	6.573 20.977 87.142 1.00 63.30	Č
		OE1 GLN D 500	6.275 21.531 86.089 1.00 63.54	Ö
		NE2 GLN D 500		N
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ATOM	7281 C ALA D 505	13.935 30.831 91.049 1.00 46.17	C
ATOM	7282 O ALA D 505	13.935 30.831 91.049 1.00 46.17 14.905 31.602 90.909 1.00 47.56	O
ATOM	7283 CB ALA D 505	11.568 31.603 90.719 1.00 43.37	. C
		13.965 29.871 91.979 1.00 46.90	N
ATOM	7285 CA GLN D 506	15.138 29.791 92.857 1.00 46.66	С
		16.398 29.604 92.040 1.00 46.13	С
ATOM	7287 O GLN D 506	17.355 30.277 92.381 1.00 46.28	0
ATOM	7288 CB GLN D 506	15.048 28.771 93.985 1.00 47.09	С
ATOM	7289 CG AGLN D 506	13.658 28.379 94.403 0.50 48.95	С
ATOM	7290 CG BGLN D 506	14.039 29.180 95.048 0.50 47.34	С
ATOM	7291 CD AGLN D 506	13.468 27.457 95.579 0.50 49.86	С
ATOM	7292 CD BGLN D 506	14.421 30.392 95.861 0.50 47.80	С
ATOM	7293 OE1AGLN D 506	14.178 26.464 95.781 0.50 49.50	0
ATOM	7294 OE1BGLN D 506	15.594 30.775 95.906 0.50 49.73	0
ATOM	7295 NE2AGLN D 506	12.458 27.779 96.403 0.50 50.31	N
ATOM	7296 NE2BGLN D 506	13.478 31.033 96.532 0.50 46.96	N
		16.442 28.769 91.020 1.00 47.10	N
		17.630 28.522 90.212 1.00 46.22	C C
		18.072 29.759 89.476 1.00 45.72	0
ATOM	7300 O LEO D 307	19.222 30.170 89.663 1.00 46.37 17.440 27.379 89.226 1.00 47.36	
ATOM	7301 CB LEU D 307	17.296 25.982 89.869 1.00 48.45	C
	7302 CO LEU D 307	17.113 24.922 88.794 1.00 48.53	C
		18.489 25.671 90.748 1.00 48.16	č
ATOM	7305 N I FILD 508	17.175 30.375 88.718 1.00 45.02	N
ATOM	7306 CA LEUD 508	17.519 31.627 88.020 1.00 43.68	С
ATOM		17.894 32.743 88.967 1.00 43.09	C
		18.818 33.502 88.632 1.00 44.39	О
		16.386 32.016 87.074 1.00 43.56	С
ATOM	7310 CG LEU D 508	16.053 30.912 86.054 1.00 43.99	С
ATOM	7311 CD1 LEU D 508	14.857 31.299 85.202 1.00 45.21	С
ATOM	7312 CD2 LEU D 508	17.215 30.636 85.129 1.00 43.98	C
	7313 N LEUD 509	17.333 32.928 90.171 1.00 41.34	N
	7314 CA LEU D 509	17.822 34.022 91.004 1.00 39.74	· C
ATOM	7315 C LEUD 509	19.286 33.882 91.406 1.00 41.27	.C
ATOM	7316 O LEUD 509	19.972 34.901 91.623 1.00 40.74	0
	7317 CB LEU D 509	16.934 34.266 92.197 1.00 38.02	С
	7318 CG LEU D 509	15.572 34.870 91.926 1.00 37.73	C
	7319 CD1 LEU D 509	14.767 34.910 93.218 1.00 39.12	C C
ATOM	7320 CD2 LEU D 509	15.677 36.266 91.374 1.00 37.20	N
ATOM	7321 N ILE D 510	19.853 32.668 91.506 1.00 42.09 21.254 32.479 91.867 1.00 41.40	C
ATOM	7322 CA ILE D 510 7323 C ILE D 510	22.109 33.098 90.761 1.00 40.98	c
ATOM	7324 O ILE D 510	23.190 33.619 91.031 1.00 40.56	0
ATOM	7325 CB ILE D 510	21.603 31.003 92.070 1.00 41.68	C
ATOM	1343 CD ILE D 310	21,003 31,003 32.070 1.00 TI.00	•

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ATOM	7326 CG1 ILE D 510	21.260 30.521 93.473 1.00 42.78	С
ATOM	7327 CG2 ILE D 510	23.086 30.720 91.924 1.00 42.12	C
ATOM	7328 CD1 ILE D 510	20.643 29.129 93.534 1.00 44.12	С
		21.639 33.084 89.512 1.00 39.99	
ATOM	7330 CA LEU D 511	22.399 33.641 88.413 1.00 40.71	С
ATOM	7331 C LEUD 511	22.747 35.095 88.658 1.00 41.31	
		23.811 35.561 88.243 1.00 42.30	0
		21.713 33.454 87.078 1.00 41.31	
ATOM	7334 CG LEU D 511	21.424 32.018 86.627 1.00 40.18	C
		20.905 32.093 85.196 1.00 40.47	C C
		22.649 31.144 86.777 1.00 38.30 21.918 35.851 89.341 1.00 41.45	N
ATOM	7338 CA SER D 512	22 208 37 220 80 606 1 00 41 06	C
ATOM	7339 C SER D 512	22.208 37.220 89.696 1.00 41.06 23.438 37.271 90.603 1.00 41.07	c
ATOM	7340 O SER D 512	24.319 38.107 90.419 1.00 42.29	O
		21.050 37.699 90.583 1.00 42.28	
		20.792 39.009 90.103 1.00 46.01	Ō
		23.516 36.375 91.602 1.00 39.13	N
		24.667 36.326 92.494 1.00 37.67	С
		25.909 35.969 91.689 1.00 37.57	С
ATOM	7346 O HIS D 513	26.965 36.614 91.811 1.00 37.05	0
		24.431 35.404 93.701 1.00 37.16	C
		23.296 36.096 94.421 0.50 37.87	
		25.455 35.520 94.790 0.50 37.66	
ATOM	7351 ND1AHIS D 513	22.007 35.629 94.434 0.50 38.32	N N
ATOM	7351 NDIDING D 513	26.189 34.437 95.249 0.50 37.48 23.271 37.255 95.114 0.50 38.08	C
ATOM	7352 CD2RHIS D 513	25.857 36.587 95.544 0.50 37.49	C
		21.235 36.493 95.087 0.50 37.64	
ATOM	7355 CE1BHIS D 513	27.001 34.839 96.222 0.50 37.37	Ċ
ATOM	7356 NE2AHIS D 513	21.983 37.457 95.547 0.50 37.37	N
		26.819 36.136 96.423 0.50 37.28	N
ATOM	7358 N ILE D 514	25.801 34.973 90.818 1.00 36.05	N
ATOM	7359 CA ILE D 514	26.949 34.627 89.996 1.00 36.78	С
	7360 C ILED 514	27.359 35.830 89.178 1.00 37.22	С
ATOM	7361 O ILED 514	28.557 36.102 89.102 1.00 37.31	0
ATOM	7362 CB ILE D 514	26.605 33.395 89.163 1.00 38.42	C
	7363 CG1 ILE D 514	26.580 32.195 90.138 1.00 38.53	C
	7364 CG2 ILE D 514	27.569 33.170 88.010 1.00 38.28	C C
ATOM ATOM	7365 CD1 ILE D 514 7366 N ARG D 515	25.727 31.080 89.564 1.00 38.48 26.461 36.624 88.596 1.00 37.86	N
	7367 CA ARG D 515	26.886 37.823 87.868 1.00 38.79	C
ATOM	7368 C ARG D 515	27.661 38.738 88.823 1.00 39.14	c
ATOM	7369 O ARG D 515	28.765 39.180 88.530 1.00 38.97	Ö
ATOM	7370 CB ARG D 515	25.698 38.606 87.335 1.00 40.22	C

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ATOM	7416 CE LYS D 520	31.685 43.833 93.425 1.00 55.68	С
ATOM	7417 NZ LYS D 520	32.165 45.060 94.170 1.00 57.32	N
	7418 N GLY D 521		N
		36.244 38.630 90.408 1.00 45.07	С
ATOM	7420 C GLY D 521	37.027 39.378 89.335 1.00 45.97	С
ATOM	7421 O GLY D 521	38.255 39.361 89.546 1.00 46.47	0
		36.453 39.964 88.263 1.00 45.24	N
		37.330 40.608 87.313 1.00 46.17	С
ATOM	7424 C MET D 522	37.977 41.811 88.008 1.00 47.57	С
	7425 O MET D 522		0
		36.883 41.251 86.040 1.00 46.68	С
ATOM	7427 CG MET D 522	35.743 40.908 85.172 1.00 47.01	С
		36.052 39.568 84.026 1.00 47.12	S
		37.801 39.701 83.767 1.00 45.10	С
		37.206 42.542 88.805 1.00 48.67	N
ATOM	7431 CA GLUD 523	37.853 43.687 89.453 1.00 49.92	С
		39.105 43.238 90.179 1.00 46.61	C
	7433 O GLUD 523		0
		36.858, 44.389, 90.334, 1.00, 56.37	
		36.040 45.451 89.644 1.00 63.92	
		36.859 46.494 88.902 1.00 68.65	
		38.084 46.628 89.154 1.00 70.98	0
		36.213 47.184 88.057 1.00 71.61	O N
		39.085 42.164 90.931 1.00 44.00 40.206 41.623 91.631 1.00 42.73	C
	7440 CA HIS D 524 7441 C HIS D 524		c
		42.462 41.370 90.874 1.00 43.70	O
		39.722 40.452 92.478 1.00 42.39	C
		40.786 39.709 93.209 1.00 42.67	
		41.535 38.688 92.672 1.00 43.20	N
		41.257 39.812 94.461 1.00 43.18	Ċ
	7447 CE1 HIS D 524	42.409 38.233 93.536 1.00 42.46	Ċ
	7448 NE2 HIS D 524	42.260 38.896 94.651 1.00 42.25	N
	7449 N LEUD 525	40.964 40.309 89.687 1.00 45.58	N
	7450 CA LEUD 525	41.967 39.726 88.807 1.00 47.55	С
	7451 C LEUD 525	42.777 40.855 88.195 1.00 50.31	С
	7452 O LEUD 525	43.968 40.797 87.964 1.00 50.79	0
ATOM	7453 CB LEUD 525	41.392 38.854 87.698 1.00 46.07	C
ATOM	7454 CG LEUD 525	42.393 38.273 86.703 1.00 44.46	С
ATOM	7455 CD1 LEU D 525	43.376 37.351 87.404 1.00 43.93	С
ATOM	7456 CD2 LEU D 525	41.671 37.541 85.593 1.00 43.69	С
ATOM	7457 N TYR D 526	42.062 41.918 87.912 1.00 53.91	N
	7458 CA TYR D 526	42.581 43.132 87.344 1.00 57.32	С
	7459 C TYR D 526	43.546 43.787 88.302 1.00 58.27	С
ATOM	7460 O TYR D 526	44.621 44.138 87.853 1.00 59.84	Ο

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ATOM	7508 N ASN D 532	51.263 43.253 89.316 1.00 85.75	N
ATOM	7509 CA ASN D 532	52.214 42.377 88.674 1.00 87.67	С
ATOM	7510 C ASN D 532	52.414 41.123 89.498 1.00 86.83	С
ATOM	7511 O ASN D 532	53.503 40.824 89.973 1.00 88.13	Ο
ATOM	7512 CB ASN D 532	53.540 43.116 88.492 1.00 91.44	С
ATOM	7513 CG ASN D 532	53.396 44.210 87.448 1.00 95.11	С
ATOM	7514 OD1 ASN D 532	52.743 43.976 86.413 1.00 96.83	Ο
ATOM	7515 ND2 ASN D 532	53.984 45.380 87.725 1.00 96.52	N
ATOM	7516 N VAL D 533	51.372 40.355 89.738 1.00 85.40	N
ATOM	7517 CA VAL D 533		С
ATOM	7518 C VAL D 533		C
ATOM	7519 O VAL D 533	51.168 36.756 89.856 1.00 84.37	Ο
ATOM	7520 CB VAL D 533	50.376 39.287 91.689 1.00 83.16	С
ATOM	7521 CG1 VAL D 533	50.469 38.081 92.594 1.00 83.74	С
ATOM	7522 CG2 VAL D 533	50.551 40.567 92.473 1.00 82.60	С
ATOM	7523 N VAL D 534	50.172 38.318 88.640 1.00 82.67	N
ATOM	7524 CA VAL D 534	49.598 37.434 87.666 1.00 81.37	С
ATOM	7525 C VAL D 534	50.520 37.295 86.464 1.00 80.71	С
ATOM	7526 O VAL D 534		Ο
ATOM	7527 CB VAL D 534	48.261 38.000 87.145 1.00 81.77	С
ATOM	7528 CG1 VAL D 534	47.647 37.281 85.967 1.00 81.40	С
ATOM	7529 CG2 VAL D 534	47.263 38.076 88.282 1.00 82.95	С
ATOM	7530 N PRO D 535	50.788 36.051 86.118 1.00 80.27	N
ATOM	7531 CA PRO D 535		С
ATOM	7532 C PRO D 535	50.835 36.148 83.705 1.00 81.79	C
ATOM	7533 O PROD 535	49.647 36.476 83.597 1.00 81.91	0
ATOM	7534 CB PRO D 535		C
ATOM	7535 CG PRO D 535	51.017 33.727 86.177 1.00 79.58	C
ATOM	7536 CD PRO D 535	50.276 34.869 86.810 1.00 80.22	С
ATOM	7537 N LEUD 536	51.630 36.118 82.638 1.00 83.19	N
ATOM	7538 CA LEU D 536		С
ATOM	7539 C LEUD 536	50.532 35.437 80.481 1.00 83.18	C
	7540 O LEUD 536	50.977 35.207 79.347 1.00 85.15	0
	7545 N TYR D 537	49.468 34.835 80.990 1.00 80.74	N
ATOM	7546 CA TYR D 537	48.744 33.854 80.189 1.00 77.68	С
ATOM	7547 C TYR D 537	47.933 34.693 79.202 1.00 75.48	C
ATOM	7548 O TYR D 537	47.192 35.577 79.597 1.00 74.48	0
ATOM	7549 CB TYR D 537	47.865 32.974 81.033 1.00 78.11	C
ATOM	7550 CG TYR D 537	48.632 32.199 82.075 1.00 78.38	C
ATOM	7551 CD1 TYR D 537	49.603 31.297 81.691 1.00 79.18	C
	7552 CD2 TYR D 537	48.385 32.348 83.424 1.00 78.50	C
ATOM	7553 CE1 TYR D 537	50.311 30.557 82.619 1.00 79.58	C
ATOM	7554 CE2 TYR D 537	49.095 31.609 84.339 1.00 78.93	C
ATOM	7555 CZ TYR D 537	50.052 30.717 83.956 1.00 79.10	C
ATOM	7556 OH TYR D 537	50.760 29.987 84.870 1.00 79.09	Ο

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ATOM	7557	N ASP D 538	48.135 34.396 77.933 1.00 73.43	N
			47.485 35.097 76.862 1.00 71.14	С
		C ASP D 538		С
		O ASP D 538		0
			48.112 34.546 75.573 1.00 76.06	С
			49.333 35.379 75.241 1.00 80.52	С
			49.297 36.609 75.511 1.00 83.41	0
		OD2 ASP D 538		Ο
ATOM	7565	N LEU D 539	45.402 33.822 76.815 1.00 61.50	N
ATOM	7566	CA LEUD 539	43.949 33.698 76.631 1.00 56.68	С
ATOM	7567	C LEU D 539	43.198 34.354 77.772 1.00 55.11	С
			42.140 34.957 77.563 1.00 54.75	Ο
			43.587 32.246 76.374 1.00 53.99	С
			42.176 31.839 76.024 1.00 51.86	С
			41.595 32.693 74.914 1.00 51.90	С
		CD2 LEU D 539		С
		N LEU D 540		N
			43.192 34.833 80.182 1.00 51.65	С
		C LEU D 540		С
		O LEU D 540		0
			43.870 34.292 81.437 1.00 49.81	C
			43.283 34.798 82.757 1.00 49.22	C
			41.996 34.063 83.099 1.00 48.02	C
		CD2 LEU D 540	44.251 34.717 83.918 1.00 47.83	C
		N LEU D 541		N
			44.461 38.378 79.526 1.00 54.36	C
		C LEU D 541		C
			42.957 39.961 78.564 1.00 55.08	0
			45.882 38.908 79.365 1.00 56.82	C C
			46.746 38.458 80.562 1.00 59.61	C
			48.213 38.814 80.410 1.00 60.75	
			46.199 38.946 81.895 1.00 59.95 43.283 38.046 77.436 1.00 52.05	C N
		N GLU D 542 CA GLU D 542	42.359 38.419 76.378 1.00 52.01	Ĉ
ATOM		CA GLU D 342 C GLU D 542	40.962 38.558 76.964 1.00 51.81	C
		O GLU D 542	40.343 39.603 76.763 1.00 52.56	ŏ
ATOM ATOM		CB GLU D 542	42.374 37.375 75.286 1.00 52.93	Č
ATOM		CG GLU D 542	41.504 37.629 74.073 1.00 54.03	Č
		CD GLU D 542		Č
ATOM		OE1 GLU D 542	43.002 36.118 73.040 1.00 56.51	o
ATOM		OE2 GLU D 542	40.862 36.198 72.325 1.00 55.79	Ö
ATOM		N MET D 543	40.460 37.558 77.678 1.00 50.53	N
ATOM		CA MET D 543	39.128 37.617 78.249 1.00 48.98	C
ATOM		C MET D 543	39.009 38.734 79.250 1.00 49.90	C
ATOM		O MET D 543	37.965 39.392 79.390 1.00 50.42	Ö
VI OIM	7001	O MILL D 343	51,705 57.572 17.570 1.00 53.12	_

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			Z78/371	_
ATOM		CB MET D 543	38.864 36.247 78.858 1.00 49.15	C
ATOM		CG MET D 543	39.038 35.161 77.798 1.00 49.35	C
ATOM		SD MET D 543	37.661 35.157 76.652 1.00 49.50	S
ATOM		CE MET D 543	38.446 35.461 75.101 1.00 50.34	C
ATOM		N LEUD 544	40.084 38.981 80.006 1.00 50.40	N
ATOM		CA LEU D 544	40.087 40.046 81.006 1.00 49.64	C
ATOM		C LEUD 544	40.020 41.371 80.274 1.00 51.52	C
ATOM		O LEUD 544	39.243 42.187 80.742 1.00 51.84	0
ATOM		CB LEU D 544	41.266 39.974 81.932 1.00 47.56	C C
ATOM		CG LEU D 544 CD1 LEU D 544	41.587 41.124 82.855 1.00 46.86 40.531 41.407 83.893 1.00 47.36	C
ATOM		CD2 LEU D 544	42.858 40.857 83.633 1.00 47.50	C
ATOM ATOM		N ASP D 545	40.742 41.598 79.188 1.00 54.73	N
ATOM		CA ASP D 545	40.657 42.868 78.490 1.00 58.31	C
ATOM		C ASP D 545	39.293 43.125 77.904 1.00 58.22	c
ATOM		O ASP D 545	38.857 44.265 77.953 1.00 58.37	ŏ
ATOM		CB ASP D 545	41.660 43.039 77.359 1.00 63.15	Č
ATOM		CG ASP D 545	43.086 43.066 77.858 1.00 68.13	č
ATOM		OD1 ASP D 545	43.347 43.145 79.089 1.00 71.17	Ō
ATOM	7621	OD2 ASP D 545	44.001 43.000 76.998 1.00 70.50	0
ATOM	7622	N ALA D 546	38.569 42.144 77.404 1.00 59.16	N
ATOM	7623	CA ALA D 546	37.246 42.333 76.848 1.00 59.75	С
ATOM	7624	C ALA D 546	36.414 43.173 77.792 1.00 61.95	С
ATOM	7625	O ALA D 546	35.707 44.069 77.382 1.00 62.80	Ο.
ATOM	7626	CB ALA D 546	36.535 41.025 76.647 1.00 59.19	С
ATOM		N HIS D 547	36.464 42.895 79.070 1.00 65.29	N
ATOM		CA HIS D 547	35.762 43.580 80.115 1.00 68.19	С
ATOM		C HIS D 547	36.237 44.968 80.398 1.00 72.31	С
ATOM		O HIS D 547	35.418 45.857 80.570 1.00 74.57	0
ATOM		CB HIS D 547	35.976 42.771 81.426 1.00 66.78	C
ATOM		CG HISD 547	34.987 41.661 81.222 1.00 65.39	C
		ND1 HIS D 547	33.769 41.664 81.821 1.00 65.32	N
		CD2 HIS D 547		C
		CE1 HIS D 547		C
		NE2 HIS D 547	33.870 39.902 80.597 1.00 65.28	N
		N ARG D 548	37.527 45.178 80.481 1.00 77.80	N C
		CA ARG D 548	38.011 46.541 80.764 1.00 83.04 37.660 47.467 79.610 1.00 83.91	C
		C ARG D 548 O ARG D 548	37.280 46.990 78.509 1.00 84.82	o
		CB ARG D 548	39.503 46.486 81.078 1.00 86.73	C
		CG ARG D 548	40.043 45.244 81.771 1.00 89.93	Č
		CD ARG D 548		C
		NE ARG D 548		N
		CZ ARG D 548		Ĉ
		NH1 ARG D 548		N
711 O1VI	, 570	1111 / INC D 370	57.500 PT.500 05.177 1.00 75.70	* 1

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ATOM 7647 NH2 ARG D 548	•	N
TER 7648 ARG D 548		
	40.094 29.783 88.544 1.00 35.42	
HETATM 7650 C2 EST D 600	39,609 28.605 87.970 1.00 37.10	С
HETATM 7651 C3 EST D 600	38.284 28.306 88.112 1.00 38.08	C
HETATM 7652 O3 EST D 600	37.791 27.149 87.568 1.00 39.71	O
	37,364 29.111 88.801 1.00 37.36	
HETATM 7654 C5 EST D 600	37.875 30.301 89.361 1.00 36.45	С
HETATM 7655 C6 EST D 600	36.954 31.006 90.323 1.00 36.00	С
HETATM 7656 C7 EST D 600	37.659 32.135 91.080 1.00 35.08	C
	38.649 32.851 90.198 1.00 33.93	
	39.773 31.877 89.830 1.00 34.03	
HETATM 7659 C10 EST D 600	39,229 30.633 89.231 1.00 34.86	С
	40.843 32.524 88.969 1.00 34.70	
	41.482 33.712 89.730 1.00 34.68	
	40.358 34.712 90.066 1.00 34.81	
HETATM 7663 C14 EST D 600	39.274 33.993 90.916 1.00 34.39	С
HETATM 7664 C15 EST D 600	38.441 35.195 91.345 1.00 35.06	C C
	39.571 36.111 91.977 1.00 34.28	
HETATM 7666 C17 EST D 600	40.746 35.820 91.048 1.00 34.55	С
HETATM /66/ 01/ EST D 600	41.355 36.988 90.563 1.00 34.28	O C
	39.825 35.299 88.774 1.00 32.87	N
	66,664 39.609 24.082 1.00 90.13 66,219 40.728 24.958 1.00 89.20	C
	67.314 41.258 25.867 1.00 88.52	c
	67.943 40.498 26.603 1.00 88.14	Ö
ATOM 7673 CP SER E 305	65.012 40.240 25.772 1.00 89.12	C
ATOM 7674 OG SER E 305	64.518 41.250 26.629 1.00 89.17	
	67.515 42.577 25.872 1.00 88.09	
ATOM 7676 CA I FILE 306	68.491 43.194 26.776 1.00 87.38	C
ATOM 7677 C LEU E 306	68.152 42.634 28.161 1.00 86.17	C
ATOM 7678 O LEU E 306	68.964 42.011 28.838 1.00 86.28	O , ,
ATOM 7679 CB LEU E 306	68.412 44.719 26.769 1.00 87.54	C
ATOM 7683 N ALAE 307	66.897 42.808 28.562 1.00 84.21	N
ATOM 7684 CA ALAE 307	66.416 42.301 29.824 1.00 82.98	С
ATOM 7685 C ALA E 307	67.160 41.033 30.203 1.00 81.72	С
ATOM 7686 O ALA E 307	67.884 41.044 31.195 1.00 81.98	0
ATOM 7687 CB ALA E 307	64.934 41.958 29.746 1.00 83.87	С
ATOM 7688 N LEUE 308	67.010 39.986 29.409 1.00 80.54	N
ATOM 7689 CA LEU E 308	67.654 38.722 29.711 1.00 80.61	С
ATOM 7690 C LEUE 308	69.161 38.703 29.707 1.00 81.30	С
ATOM 7691 O LEUE 308	69.724 37.659 30.049 1.00 82.75	O
ATOM 7692 CB LEU E 308	67.085 37.650 28.782 1.00 80.17	С
ATOM 7693 CG LEU E 308	65.577 37.475 28.851 1.00 81.19	С
ATOM 7694 CD1 LEU E 308	65.154 36.148 28.222 1.00 81.69	C

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ATOM	7695	CD2 LEU E 308	65.053 37.544 30.286 1.00 81.62	С
ATOM	7696	N SER E 309		N
ATOM	7697	CA SER E 309	71.347 39.770 29.359 1.00 80.22	С
ATOM	7698	C SER E 309	71.999 40.597 30.445 1.00 78.84	С
ATOM	7699	O SER E 309	73.155 40.377 30.811 1.00 79.47	0
ATOM	7700	CB SER E 309	71.753 40.479 28.045 1.00 81.59	С
ATOM	7701	OG SER E 309	70.952 39.844 27.041 1.00 84.79	0
ATOM	7702	N LEUE 310	71.283 41.600 30.940 1.00 77.00	N
ATOM	7703	CA LEU E 310	71.887 42.438 31.972 1.00 74.38	С
ATOM	7704	C LEUE310	72.143 41.592 33.215 1.00 72.92	С
ATOM	7705	O LEUE 310	71.526 40.578 33.479 1.00 72.38	Ο
ATOM	7706	CB LEUE 310	71.076 43.676 32.277 1.00 73.94	С
ATOM	7707	CG LEUE 310	70.244 44.241 31.131 1.00 73.26	С
ATOM	7708	CD1 LEU E 310	68.782 44.089 31.487 1.00 73.44	С
ATOM	7709	CD2 LEU E 310	70.608 45.687 30.897 1.00 74.10	С
ATOM	7710	N THRE311	73.126 42.065 33.953 1.00 71.49	N
ATOM	7711	CA THRE 311	73.553 41.413 35.178 1.00 70.53	С
ATOM	7712	C THRE311	72.746 42.059 36.275 1.00 69.73	С
ATOM	7713	O THRE311	72.361 43.205 36.053 1.00 68.45	0
ATOM	7714	CB THRE311	75.062 41.619 35.335 1.00 71.32	С
			75.457 42.979 35.545 1.00 71.11	0
ATOM	7716	CG2 THR E 311	75.761 41.156 34.061 1.00 71.58	С
ATOM	7717	N ALA E 312	72.529 41.428 37.424 1.00 69.88	N
ATOM		CA ALAE 312		С
ATOM	7719	C ALA E 312	72.166 43.487 38.671 1.00 69.88	С
		O ALA E 312		0
ATOM	7721	CB ALAE312	71.763 41.300 39.794 1.00 69.72	С
ATOM		N ASP E 313		N
ATOM			73.901 45.138 38.782 1.00 72.48	C
		C ASP E 313		С
			72.943 47.120 38.016 1.00 69.52	0
			75.426 45.194 38.920 1.00 76.80	С
			75.762 44.768 40.352 1.00 80.77	С
		OD1 ASP E 313	75.182 45.405 41.270 1.00 82 .19	0
		OD2 ASP E 313	76.567 43.816 40.553 1.00 82.97	0
		N GLN E 314	73.457 45.680 36.414 1.00 69.29	N
		CA GLNE 314	72.996 46.542 35.335 1.00 69.21	С
ATOM		C GLNE314	71.491 46.761 35.419 1.00 67.65	С
		O GLN E 314	71.014 47.872 35.215 1.00 68.31	О
		CB GLNE 314	73.320 45.959 33.960 1.00 71.55	C
		CG GLNE 314	74.627 45.191 33.998 1.00 74.36	C
		CD GLNE 314	75.069 44.694 32.649 1.00 76.01	C
		OE1 GLN E 314	74.981 43.502 32.343 1.00 77.18	0
		NE2 GLN E 314	75.541 45.682 31.887 1.00 77.10	N
ATOM	7739	N METE 315	70.760 45.697 35.720 1.00 64.89	N

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ATOM	7740 CA MET E 315	69.321 45.727 35.900 1.00 61.52	С
ATOM	7741 C MET E 315	68.984 46.796 36.941 1.00 60.15	С
ATOM	7742 O MET E 315	68.232 47.738 36.694 1.00 59.18	Ο
ATOM	7743 CB MET E 315	68.866 44.369 36.399 1.00 61.20	С
ATOM	7744 CG MET E 315	67.374 44.157 36.557 1.00 61.73	С
ATOM	7745 SD MET E 315	66.545 43.770 34.975 1.00 60.72	S
ATOM	7746 CE MET E 315	65.521 45.250 34.944 1.00 61.58	С
ATOM	7747 N VALE 316	69.586 46.706 38.128 1.00 59.06	N
ATOM	7748 CA VALE 316	69.334 47.693 39.160 1.00 58.51	С
ATOM	7749 C VALE 316	69.568 49.109 38.668 1.00 59.26	С
ATOM	7750 O VALE 316	68.757 49.996 38.917 1.00 60.99	О
ATOM	7751 CB VALE 316	70.182 47.522 40.426 1.00 57.64	С
ATOM	7752 CG1 VAL E 316	69.926 48.654 41.412 1.00 56.70	С
ATOM	7753 CG2 VAL E 316	69.871 46.177 41.069 1.00 57.96	С
ATOM	7754 N SER E 317	70.665 49.373 38.003 1.00 59.51	N
ATOM	7755 CA SER E 317	70.944 50.739 37.560 1.00 60.83	С
ATOM	7756 C SER E 317	70.009 51.159 36.456 1.00 59.74	С
ATOM	7757 O SER E 317	69.545 52.304 36.418 1.00 60.86	Ο
ATOM	7758 CB SER E 317	72.391 50.810 37.057 1.00 62.92	С
ATOM	7759 OG SER E 317	72.768 49.429 36.981 1.00 66.28	Ο
ATOM	7760 N ALA E 318	69.718 50.225 35.560 1.00 57.32	N
ATOM	7761 CA ALA E 318	68.783 50.552 34.489 1.00 55.79	С
ATOM	7762 C ALA E 318	67.476 51.078 35.083 1.00 55.92	С
ATOM	7763 O ALA E 318	66.890 52.070 34.648 1.00 55.88	0
ATOM	7764 CB ALA E 318	68.486 49.293 33.718 1.00 55.78	С
ATOM	7765 N LEUE 319	66.998 50.370 36.111 1.00 55.08	N
ATOM	7766 CA LEUE 319	65.771 50.688 36.813 1.00 52.78	С
ATOM	7767 C LEUE 319	65.972 51.959 37.583 1.00 54.13	C
ATOM	7768 O LEUE 319	65.170 52.873 37.500 1.00 54.67	0
ATOM		65.441 49.546 37.767 1.00 50.55	C
ATOM		64.947 48.274 37.072 1.00 49.71	C
	7771 CD1 LEU E 319	64.666 47.218 38.123 1.00 48.77	C
	7772 CD2 LEU E 319	63.747 48.565 36.173 1.00 48.75	C
	7773 N LEUE 320	67.090 52.082 38.278 1.00 56.12	N
	7774 CA LEUE 320	67.366 53.288 39.055 1.00 58.13	С
	7775 C LEUE 320	67.378 54.490 38.144 1.00 60.62	C
	7776 O LEUE 320	67.002 55.584 38.522 1.00 62.27	0
	7777 CB LEUE 320	68.697 53.147 39.799 1.00 57.11	C
	7778 CG LEUE 320	68.449 52.587 41.195 1.00 56.24	C
	7779 CD1 LEU E 320	69.771 52.365 41.887 1.00 57.34	C
	7780 CD2 LEU E 320	67.526 53.555 41.901 1.00 55.80	C
	7781 N ASP E 321	67.814 54.306 36.919 1.00 63.78	N
		67.844 55.362 35.948 1.00 67.74	С
	7783 C ASP E 321	66.504 55.768 35.388 1.00 66.51	C
ATOM	7784 O ASP E 321	66.284 56.942 35.112 1.00 68.09	0

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ATOM	7785	CB ASP E 321	68.660 54.866 34.732 1.00 73.25	С
ATOM	7786	CG ASP E 321	70.007 55.573 34.820 1.00 78.83	С
ATOM	7787	OD1 ASP E 321	70.229 56.287 35.842 1.00 81.54	0
ATOM	7788	OD2 ASP E 321	70.810 55.390 33.871 1.00 81.74	0
ATOM	7789	N ALA E 322	65.596 54.825 35.185 1.00 63.63	N
ATOM	7790	CA ALAE 322	64.310 55.135 34.587 1.00 60.60	С
ATOM	7791	C ALA E 322	63.429 55.954 35.499 1.00 59.85	С
ATOM	7792	O ALA E 322	62.408 56.514 35.072 1.00 59.85	Ο
ATOM	7793	CB ALAE 322	63.663 53.798 34.246 1.00 60.27	С
ATOM	7794	N GLU E 323	63.770 56.023 36.786 1.00 58.01	N
ATOM	7795	CA GLUE 323	62.919 56.750 37.730 1.00 55.97	С
ATOM	7796	C GLU E 323	62.490 58.058 37.151 1.00 55.08	С
ATOM	7797	O GLU E 323	63.247 58.786 36.523 1.00 57.54	Ο
ATOM	7798	CB GLUE 323	63.694 56.817 39.039 1.00 55.76	С
ATOM	7799	CG GLUE 323	63.544 55.500 39.811 1.00 55.81	С
ATOM	7800	CD GLUE 323	62.152 55.434 40.397 1.00 56.70	С
ATOM	7801	OE1 GLU E 323	61.776 56.308 41.211 1.00 57.38	Ο
ATOM	7802	OE2 GLU E 323	61.381 54.527 40.053 1.00 57.03	Ο
ATOM	7803	N PRO E 324	61.243 58.415 37.306 1.00 54.39	N
ATOM	7804	CA PROE 324	60.676 59.671 36.823 1.00 53.99	С
	7805	C PRO E 324	61.006 60.793 37.785 1.00 53.72	С
ATOM	7806	O PRO E 324	61.466 60.572 38.900 1.00 55.05	0
		CB PROE 324	59.153 59.457 36.810 1.00 53.22	С
		CG PROE 324	59.024 58.476 37.934 1.00 53.17	C
ATOM	7809	CD PROE 324	60.264 57.627 38.049 1.00 53.88	С
		N PRO E 325	60.760 62.008 37.397 1.00 53.96	N
		CA PROE 325	60.981 63.188 38.208 1.00 55.99	С
		C PRO E 325	59.956 63.279 39.316 1.00 57.54	С
		O PRO E 325		О
		CB PROE 325		С
		CG PROE 325		C -
		CD PROE 325	60.207 62.331 36.081 1.00 54.93	С
		N ILE E 326	60.110 64.010 40.390 1.00 59.40	N
ATOM		CA ILEE 326	59.047 64.094 41.405 1.00 62.16	С
		C ILE E 326	58.231 65.358 41.070 1.00 60.95	C
		O ILE E 326	58.865 66.421 40.958 1.00 61.11	0
		CB ILE E 326	59.425 64.267 42.892 1.00 64.57	С
		CG1 ILE E 326	60.372 65.455 43.142 1.00 67.03	С
		CG2 ILE E 326	60.016 62.999 43.511 1.00 64.53	C
		CD1 ILE E 326	61.627 65.591 42.290 1.00 69.10	С
ATOM		N LEUE 327	56.928 65.259 40.897 1.00 59.14	N
ATOM		CA LEUE 327	56.176 66.473 40.595 1.00 57.57	С
ATOM		C LEUE 327	55.911 67.247 41.875 1.00 58.33	C
		O LEU E 327	56.166 66.834 42.999 1.00 57.32	0
ATOM	7829	CB LEUE 327	54.907 66.051 39.874 1.00 56.25	С

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ATOM	7830 CG	LEU E 327	55.062 65.113 38.692 1.00 55.77	С
ATOM	7831 CD	1 LEU E 327	53.826 65.144 37.802 1.00 55.31	С
ATOM	7832 CD2	2 LEU E 327	56.305 65.426 37.874 1.00 55.58	С
ATOM	7833 N	TYR E 328	55.396 68.458 41.735 1.00 60.55	N
ATOM		TYR E 328	55.008 69.326 42.832 1.00 62.06	С
ATOM	7835 C	TYR E 328	53.498 69.533 42.642 1.00 63.12	C
ATOM	7836 O	TYR E 328	53.050 69.583 41.495 1.00 62.44	0
ATOM	7837 CB	TYR E 328	55.674 70.709 42.851 1.00 62.29	С
ATOM	7838 CG	TYR E 328	57.079 70.585 43.383 1.00 62.82	С
ATOM	7839 CD	1 TYR E 328	57.303 70.581 44.747 1.00 63.59	С
ATOM	7840 CD2	2 TYR E 328	58.168 70.444 42.546 1.00 63.07	С
ATOM	7841 CE	TYR E 328	58.587 70.447 45.235 1.00 64.17	С
ATOM	7842 CE2	2 TYR E 328	59.455 70.304 43.031 1.00 63.49	С
ATOM	7843 CZ	TYR E 328	59,657 70.302 44.386 1.00 64.13	С
ATOM	7844 OH	TYR E 328	60.928 70.165 44.899 1.00 65.08	Ο
ATOM	7845 N	SER E 329	52.766 69.635 43.728 1.00 65.10	N
ATOM	7846 CA	SER E 329	51.337 69.839 43.584 1.00 67.67	C
ATOM	7847 C	SER E 329	51.090 71.276 43.149 1.00 70.67	C
ATOM	7848 O	SER E 329	51.825 72.164 43.562 1.00 70.24	Ο
ATOM	7849 CB	SER E 329	50.621 69.568 44.903 1.00 66.71	С
ATOM	7850 OG	SER E 329	49.353 70.169 44.764 1.00 67.28	Ο
ATOM	7851 N	GLU E 330	50.068 71.489 42.340 1.00 75.59	N
ATOM	7852 CA	GLUE 330	49.667 72.797 41.847 1.00 79.74	С
ATOM	7853 C	GLU E 330	49.227 73.680 43.009 1.00 80.39	С
ATOM	7854 O	GLU E 330	48.555 73.276 43.957 1.00 80.63	Ο
ATOM	7855 CB	GLU E 330	48.524 72.672 40.843 1.00 83.66	С
ATOM		GLU E 330	47.189 73.282 41.204 1.00 88.63	С
ATOM	7857 CD	GLU E 330	46.072 72.327 41.592 1.00 91.97	С
ATOM	7858 OE	1 GLU E 330	45.391 71.767 40.683 1.00 93.20	0
ATOM	7859 OE	2 GLU E 330	45.821 72.110 42.814 1.00 93.64	0
ATOM		PHE E 337		N
ATOM	7861 CA	PHE E 337	40.117 71.718 51:376 1.00 84.72	С
		PHE E 337	38.650 71.308 51.477 1.00 83.52	C
ATOM	7863 O	PHE E 337	38.042 71.506 52.526 1.00 84.39	0
ATOM	7864 CB	PHE E 337	40.874 70.727 52.265 1.00 85.39	C
ATOM	7865 CG	PHE E 337	42.298 70.544 51.823 1.00 86.55	C
ATOM		1 PHE E 337	42.658 70.658 50.496 1.00 87.08	C
ATOM		2 PHE E 337	43.280 70.276 52.755 1.00 87.08	C
ATOM		1 PHE E 337	43.966 70.504 50.112 1.00 87.85	C
MOTA		2 PHE E 337	44.588 70.119 52.384 1.00 87.59	С
ATOM		PHE E 337	44.932 70.231 51.053 1.00 88.06	C
ATOM		SER E 338	38.134 70.743 50.400 1.00 80.45	N
ATOM		SER E 338	36.748 70.299 50.424 1.00 77.39	C
ATOM		SER E 338	36.773 69.014 49.635 1.00 75.91	C
ATOM	7874 O	SER E 338	37.700 68.892 48.837 1.00 76.77	O

45.125 66.730 43.455 1.00 50.99

ATOM 7919 C LEUE 345

ATOM 7920 O LEUE 345 46,007 66.515 42,626 1.00 49.85 O C 45.081 68.394 45.131 1.00 53.85 ATOM 7921 CB LEU E 345 ATOM 7922 CG LEUE 345 44.953 69.833 45.603 1.00 56.56 C C 44.136 69.811 46.891 1.00 57.16 ATOM 7923 CD1 LEU E 345 C ATOM 7924 CD2 LEU E 345 46.313 70.472 45.781 1.00 56.83 ATOM 7925 N LEUE 346 44.571 65.814 44.258 1.00 49.14 N C 44.986 64.418 44.177 1.00 47.49 ATOM 7926 CA LEU E 346 ATOM 7927 C LEU E 346 44.896 63.900 42.760 1.00 46.79 C ATOM 7928 O LEUE 346 45.813 63.355 42.149 1.00 45.83 0 C ATOM 7929 CB LEUE 346 44.110 63.680 45.186 1.00 47.01 C ATOM 7930 CG LEU E 346 44.533 63.926 46.634 1.00 47.91 ATOM 7931 CD1 LEU E 346 43.936 62.861 47.554 1.00 47.78 C ATOM 7932 CD2 LEU E 346 46.047 63.950 46.838 1.00 47.51 C N 43.722 64.101 42.185 1.00 45.98 ATOM 7933 N THR E 347 43.387 63.697 40.825 1.00 45.47 C ATOM 7934 CA THR E 347 44,236 64,394 39,803 1.00 46.07 C ATOM 7935 C THR E 347 44.710 63.770 38.859 1.00 46.31 0 ATOM 7936 O THR E 347 C 41.876 63.928 40.726 1.00 45.77 ATOM 7937 CB THR E 347 41.285 62.634 40.511 1.00 46.10 0 ATOM 7938 OG1 THR E 347 41.473 64.979 39.747 1.00 45.14 C ATOM 7939 CG2 THR E 347 ATOM 7940 N ASN E 348 44,512 65,679 39,952 1.00 47,18 N C 45.376 66.434 39.055 1.00 47.33 ATOM 7941 CA ASN E 348 C 46.804 65.869 39.095 1.00 45.16 ATOM 7942 C ASN E 348 47.477 65.591 38.118 1.00 44.24 0 ATOM 7943 O ASN E 348 C ATOM 7944 CB ASN E 348 45,386 67.899 39.504 1.00 50.18 C ATOM 7945 CG ASN E 348 46.348 68.766 38.697 1.00 54.12 0 47,532 69,034 39,065 1,00 54,75 ATOM 7946 OD1 ASN E 348 ATOM 7947 ND2 ASN E 348 45.771 69.187 37.550 1.00 54.87 N 47.335 65.683 40.286 1.00 43.41 N ATOM 7948 N LEUE 349 48,674 65.173 40.501 1.00 42.15 C ATOM 7949 CA LEU E 349 ATOM 7950 C LEUE 349 C 48.756 63.811 39.856 1.00 42.03 49.757 63.555 39.179 1.00 43.04 O٠ ATOM 7951 O LEUE 349 48.968 65.152 42.004 1.00 42.95 C ATOM 7952 CB LEU E 349 C 50.340 64.653 42.411 1.00 43.25 ATOM 7953 CG LEU E 349 51.417 65.586 41.855 1.00 43.86 C ATOM 7954 CD1 LEU E 349 C 50.481 64.509 43.905 1.00 43.16 ATOM 7955 CD2 LEU E 349 N ATOM 7956 N ALA E 350 47.759 62.935 40.017 1.00 40.82 C 47.776 61.615 39.414 1.00 39.79 ATOM 7957 CA ALA E 350 C 47.854 61.751 37.900 1.00 41.20 ATOM 7958 C ALA E 350 ATOM 7959 O ALA E 350 48.729 61.187 37.235 1.00 41.18 0 46.545 60.810 39.745 1.00 39.02 C ATOM 7960 CB ALA E 350 46,952 62,556 37,331 1.00 42.05 N ATOM 7961 N ASP E 351 46,960 62,747 35.894 1.00 43.55 C ATOM 7962 CA ASP E 351 ATOM 7963 C ASP E 351 48,325 63,146 35,367 1.00 44.64 C 48.749 62.760 34.258 1.00 45.95 0 ATOM 7964 O ASP E 351

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ΔΤΩΜ	7065 CR ASP F 351	45 802 <i>63 754</i> 35 534 1 00 45 99	С
ATOM	7966 CG ASP E 351	45.849 63.920 34.033 1.00 49.35	Č
ATOM	7967 OD1 ASP E 351	45.353 63.008 33.355 1.00 51.07	0
ATOM	7968 OD2 ASP E 351	46.340 64.968 33.562 1.00 51.79	0
ATOM	7969 N ARGE 352	49.084 63.941 36.102 1.00 44.28	N
ATOM	7970 CA ARG E 352	50.397 64.373 35.671 1.00 44.89	С
		51.454 63.293 35.758 1.00 45.67	
ATOM	7972 O ARGE 352	52.277 63.094 34.847 1.00 46.39	0
ATOM	7973 CB ARG E 352	50.791 65.599 36.479 1.00 45.31 50.074 66.823 35.923 1.00 47.04	C
ATOM	7974 CG ARG E 352	50.074 66.823 35.923 1.00 47.04	C
ATOM	7975 CD ARG E 352	51.018 68.022 36.145 1.00 48.79	C
ATOM	7976 NE ARG E 352	50.749 68.361 37.541 1.00 51.41	N
ATOM	7977 CZ ARGE 352	51.710 68.620 38.432 1.00 52.42	C
ATOM	7978 NHI ARG E 352	52.973 68.607 38.039 1.00 51.54	N
		51.239 68.883 39.656 1.00 53.39	
	7980 N GLUE 353	51.452 62.533 36.853 1.00 44.89 52.427 61.455 36.998 1.00 42.61	
		52.225 60.407 35.922 1.00 41.58	
		53.165 59.738 35.520 1.00 41.66	
		52.212 60.810 38.359 1.00 42.28	
ATOM	7985 CG GLUE 353	52.159 61.796 39.504 1.00 42.55	Č
ATOM	7986 CD GLUE 353	52.159 61.796 39.504 1.00 42.55 52.357 61.064 40.813 1.00 44.11	Ċ
ATOM	7987 OE1 GLU E 353	53.418 60.438 40.997 1.00 44.30	0
		51.435 61.111 41.652 1.00 45.63	
		50.992 60.243 35.461 1.00 41.20	
		50.638 59.265 34.459 1.00 41.40	
		51.483 59.446 33.222 1.00 41.40	
ATOM	7992 O LEUE 354	51.988 58.492 32.637 1.00 41.35	0
ATOM	7993 CB LEU E 354	49.132 59.282 34.178 1.00 40.94 48.423 58.370 35.199 1.00 40.08	C
ATOM	7994 CG LEUE 354	48.423 58.370 35.199 1.00 40.08	С
		46.976 58.751 35.290 1.00 39.80	C
		48.644 56.929 34.750 1.00 40.20	C N
		51.649 60.702 32.847 1.00 41.94 52.492 60.999 31.680 1.00 42.07	C
	7998 CA VALE 355 7999 C VALE 355	53.888 60.446 31.901 1.00 43.39	C ·
	8000 O VALE 355	54.390 59.614 31.137 1.00 45.00	Ö
	8001 CB VALE 355	52.519 62.515 31.489 1.00 39.86	C
		53.353 62.849 30.312 1.00 40.48	C
		51.096 62.910 31.194 1.00 41.98	C
		54.552 60.832 32.977 1.00 43.36	N
		55.870 60.352 33.297 1.00 44.05	С
	8006 C HIS E 356	55.863 58.844 33.379 1.00 43.90	С
ATOM	8007 O HIS E 356	56.805 58.186 32.912 1.00 43.40	Ο
		56.329 61.010 34.606 1.00 48.13	С
ATOM	8009 CG HIS E 356	56.461 62.483 34.331 1.00 51.56	С

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	57 (6 (2) 11) 24 140 1 00 53 20	N
ATOM 8010 ND1 HIS E 356		C
ATOM 8011 CD2 HIS E 356		C
ATOM 8012 CE1 HIS E 356		N
ATOM 8013 NE2 HIS E 356		N
ATOM 8014 N MET E 357 ATOM 8015 CA MET E 357		Ċ
ATOM 8015 CA MET E 357	_	c
ATOM 8016 C MET E 357 ATOM 8017 O MET E 357		Ö
ATOM SOLE CR MET E 357	53.379 56.351 34.719 1.00 42.21	C
ATOM SOIS CE METE 357	53.567 54.845 35.039 1.00 41.81	C
ATOM 8020 SD MET F 357	52.012 54.208 35.644 1.00 41.75	S
ATOM 8021 CF MET E 357	51.933 55.033 37.233 1.00 43.97	С
ATOM 8022 N ILEE 358	54.191 56.505 31.800 1.00 42.02	N
ATOM 8023 CA ILE E 358	54.262 55.912 30.473 1.00 41.51	С
ATOM 8024 C ILE E 358		С
ATOM 8025 O ILE E 358	56.154 54.908 29.485 1.00 42.86	O .
ATOM 8026 CB ILE E 358	53.376 56.704 29.491 1.00 39.37	C
ATOM 8027 CG1 ILE E 358	51.923 56.606 29.934 1.00 38.89	С
ATOM 8028 CG2 ILE E 358	53.525 56.159 28.096 1.00 38.83	С
ATOM 8029 CD1 ILE E 358	50.944 57.324 29.059 1.00 38.55	С
ATOM 8030 N ASN E 359	56.391 57.053 30.131 1.00 44,20	N
	57.787 57.136 29.737 1.00 46.66	C
ATOM 8032 C ASN E 359		C
ATOM 8033 O ASN E 359	59.451 55.383 29.997 1.00 46.33	0
ATOM 8034 CB ASN E 359	58.293 58.549 30.031 1.00 51.90	C C
ATOM 8035 CG ASN E 359	57.759 59.447 28.926 1.00 55.87	0
ATOM 8036 ODI ASNE 359	58.138 59.117 27.792 1.00 59.61	N,
	56.958 60.463 29.184 1.00 56.96 58.512 56.147 31.823 1.00 44.28	N
ATOM 8038 N TRP E 360		C
	59.254 55.214 32.656 1.00 42.84 59.039 53.781 32.220 1.00 42.98	c
ATOM 8040 C TRP E 360 ATOM 8041 O TRP E 360		Ö
ATOM 8041 O TRP E 360 ATOM 8042 CB TRP E 360		C
ATOM 8042 CB TRI E 360 ATOM 8043 CG TRP E 360		C
ATOM 8044 CD1 TRP E 360		С
ATOM 8045 CD2 TRP E 360		С
ATOM 8046 NE1 TRP E 360		N
ATOM 8047 CE2 TRP E 360		С
ATOM 8048 CE3 TRP E 360		С
ATOM 8049 CZ2 TRP E 360		С
ATOM 8050 CZ3 TRP E 360	56.453 51.623 35.608 1.00 43.00	С
ATOM 8051 CH2 TRP E 360	57.261 50.814 36.418 1.00 42.73	С
ATOM 8052 N ALA E 361	57.799 53.369 31.978 1.00 44.16	N
ATOM 8053 CA ALA E 361		C
ATOM 8054 C ALA E 361	58.326 51.629 30.391 1.00 45.81	С

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ATOM	8055 O ALA E 361		0
		55.998 51.877 31.146 1.00 43.81	C
ATOM	8057 N LYS E 362	58.497 52.519 29.414 1.00 48.10	N
ATOM	8058 CA LYS E 362	59.294 52.228 28.240 1.00 51.06	C
	8059 C LYS E 362		С
	8060 O LYS E 362		0
		59.220 53.381 27.248 1.00 52.88	С
ATOM	8062 CG LYS E 362	57.815 53.499 26.670 1.00 56.32	С
ATOM	8063 CD LYS E 362	57.545 52.350 25.706 1.00 59.44	С
ATOM	8064 CE LYS E 362	56.994 52.840 24.368 1.00 62.09	C
ATOM	8065 NZ LYS E 362	56.986 51.784 23.287 1.00 63.02	
ATOM	8066 N ARG E 363	61.327 52.195 29.615 1.00 52.40	N
		62.665 51.847 30.003 1.00 53.85	С
	8068 C ARG E 363		C
	8069 O ARG E 363		0
	8070 CB ARG E 363		C
		62.449 54.263 30.564 1.00 62.85	C
ATOM	8072 CD ARG E 363	62.981 54.929 29.283 1.00 68.62	C
ATOM	8073 NE ARGE 363	64.337 55.368 29.657 1.00 74.45	N C
ATOM	8074 CZ ARGE 363	64.512 56.355 30.546 1.00 77.99	N
		63.433 56.948 31.074 1.00 79.59	N N
	8076 NH2 ARG E 363 8077 N VAL E 364	65.754 56.721 30.882 1.00 79.71 61.687 49.981 31.340 1.00 51.00	N
	8078 CA VALE 364		C.
	8079 C VALE 364		c
		61.613 47.311 30.477 1.00 48.86	Ö
ATOM	8080 C VAL E 364	60.540 48.512 32.969 1.00 47.56	C
ATOM	8082 CG1 VAL E 364	60.553 47.172 33.659 1.00 45.31	C
		60.173 49.655 33.902 1.00 47.17	C
		63.501 47.189 31.585 1.00 47.26	N
		64.060 46.117 30.774 1.00 47.42	C
	8086 C PRO E 365	63.036 45.052 30.471 1.00 48.06	С
	8087 O PRO E 365	62.452 44.562 31.429 1.00 48.89	0
	8088 CB PRO E 365	65.247 45.558 31.568 1.00 47.14	C
ATOM	8089 CG PRO E 365	65.708 46.873 32.187 1.00 48.39	C
	8090 CD PRO E 365	64.443 47.641 32.608 1.00 48.24	С
	8091 N GLY E 366	62.811 44.736 29.191 1.00 48.05	N
	8092 CA GLY E 366	61.888 43.705 28.785 1.00 46.86	C
	8093 C GLY E 366	60.530 44.191 28.352 1.00 47.67	C
	8094 O GLY E 366	59.827 43.546 27.556 1.00 48.69	0
	8095 N PHE E 367	60.102 45.339 28.867 1.00 47.11	N
	8096 CA PHE E 367	58.791 45.899 28.567 1.00 46.48	C
	8097 C PHE E 367	58.503 46.101 27.083 1.00 46.37	C
	8098 O PHE E 367	57.541 45.719 26.424 1.00 45.46	0
ATOM	8099 CB PHE E 367	58.659 47.258 29.288 1.00 45.29	С

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ATOM	8100	CG PHE E 367		С
		CD1 PHE E 367		С
		CD2 PHE E 367	56.941 48.862 28.393 1.00 46.15	С
ATOM	8103	CE1 PHE E 367	54.949 47.675 29.873 1.00 45.31	С
		CE2 PHE E 367	55.650 49.347 28.314 1.00 46.17	С
ATOM	8105	CZ PHE E 367	54.648 48.755 29.064 1.00 45.75	С
ATOM	8106	N VAL E 368	59.433 46.793 26.454 1.00 46.85	N
ATOM	8107	CA VALE 368	59.418 47.174 25.063 1.00 47.56	С
ATOM	8108	C VAL E 368	59.401 45.970 24.147 1.00 49.50	С
ATOM	8109	O VAL E 368	58.958 46.117 22.986 1.00 51.13	0
ATOM	8110	CB VALE 368	60.621 48.100 24.855 1.00 46.24	С
		CG1 VAL E 368	61.431 47.684 23.666 1.00 46.91	C
		CG2 VAL E 368	60.060 49.501 24.798 1.00 46.71	С
		N ASP E 369	59.830 44.797 24.609 1.00 49.22	N
			59.748 43.611 23.791 1.00 49.90	C
		C ASP E 369		C
		O ASP E 369		0
			60.551 42.440 24.356 1.00 53.57	C C
		CG ASP E 369	62.001 42.767 24.627 1.00 57.64	0
		OD1 ASP E 369	62.632 43.529 23.837 1.00 59.82	0
		OD2 ASP E 369	62.486 42.232 25.664 1.00 58.81 57.282 43.617 24.298 1.00 46.26	N
		N LEUE 370		C
		CA LEUE 370 C LEUE 370		c
		O LEUE 370		ő
			55.220 43.372 25.525 1.00 44.62	C
			55.824 42.653 26.729 1.00 43.72	Č
			55.091 42.990 28.001 1.00 43.76	C
ATOM	8128	CD2 LEU E 370	55.711 41.158 26.484 1.00 44.23	C
			54.118 43.310 22.554 1.00 42.71	N
			53.471 44.056 21.474 1.00 42.93	С
		C THR E 371	52.959 45.372 21.994 1.00 43.15	С
ATOM	8132	O THR E 371	52.609 45.480 23.152 1.00 42.85	Ο
ATOM	8133	CB THR E 371	52.262 43.256 20.975 1.00 43.47	С
ATOM	8134	OG1 THR E 371	51.545 42.926 22.173 1.00 44.71	О
		CG2 THR E 371	52.704 41.986 20.277 1.00 43.38	С
		N LEU E 372	52.865 46.372 21.118 1.00 45.22	N
		CA LEUE 372	52.359 47.690 21.532 1.00 44.77	C
		C LEU E 372	51.069 47.563 22.338 1.00 45.09	C
		O LEU E 372	50.957 48.200 23.398 1.00 44.44	0
		CB LEUE 372	52.234 48.576 20.295 1.00 42.49	C
		CG LEU E 372	53.548 48.903 19.617 1.00 41.22	C
		CD1 LEU E 372	53.264 49.684 18.350 1.00 43.25	C
			54.427 49.746 20.512 1.00 41.76	C
ATUM	8144	N HIS E 373	50.106 46.745 21.912 1.00 45.43	N

C ` 48.884 46.647 22.706 1.00 47.32 ATOM 8145 CA HIS E 373 ATOM 8146 C HISE 373 49.173 46.044 24.067 1.00 47.30 48.655 46.557 25.084 1.00 46.34 ATOM 8147 O HISE 373 O ATOM 8148 CB HIS E 373 47.801 45.952 21.902 1.00 49.96 C 47.251 46.889 20.863 1.00 53.52 C ATOM 8149 CG HIS E 373 47.573 46.867 19.519 1.00 54.14 N ATOM 8150 ND1 HIS E 373 46.370 47.908 21.001 1.00 54.57 C ATOM 8151 CD2 HIS E 373 C ATOM 8152 CE1 HIS E 373 46.907 47.824 18.904 1.00 54.87 ATOM 8153 NE2 HIS E 373 46.166 48.494 19.778 1.00 55.54 N ATOM 8154 N ASP E 374 50.019 45.003 24.138 1.00 46.26 N ATOM 8155 CA ASP E 374 50.307 44.485 25.479 1.00 46.26 C 50,909 45,514 26,420 1,00 45,67 ATOM 8156 C ASP E 374 C ATOM 8157 O ASP E 374 50.611 45.500 27.626 1.00 45.81 0 ATOM 8158 CB ASP E 374 51.139 43.207 25.389 1.00 47.09 C ATOM 8159 CG ASP E 374 50.122 42.191 24.898 1.00 49.52 C ATOM 8160 OD1 ASP E 374 48.918 42.529 24.963 1.00 49.64 0 ATOM 8161 OD2 ASP E 374 50.503 41.088 24.455 1.00 53.31 0 ATOM 8162 N GLN E 375 51.740 46.411 25.899 1.00 44.54 N ATOM 8163 CA GLN E 375 52.289 47.443 26.773 1.00 44.93 C C ATOM 8164 C GLN E 375 51.124 48.252 27.326 1.00 45.36 ATOM 8165 O GLN E 375 50.974 48.358 28.552 1.00 46.12 0 ATOM 8166 CB GLN E 375 53.267 48.293 25.992 1.00 44.78 C ATOM 8167 CG GLN E 375 54.412 47.413 25.523 1.00 46.26 C C ATOM 8168 CD GLN E 375 55.356 48.147 24.606 1.00 46.81 55.540 49.358 24.681 1.00 47.74 0 ATOM 8169 OE1 GLN E 375 ATOM 8170 NE2 GLN E 375 55.949 47.353 23.742 1.00 47.03 N 50.261 48.767 26.442 1.00 44.88 N ATOM 8171 N VALE 376 ATOM 8172 CA VALE 376 49.094 49.513 26.906 1.00 43.54 C ATOM 8173 C VALE 376 C 48.332 48.676 27.929 1.00 43.22 ATOM 8174 O VALE 376 0 47.948 49.192 28.975 1.00 43.63 ATOM 8175 CB VALE 376 48.174 49.957 25.768 1.00 43.24 C ATOM 8176 CG1 VAL E 376 47.227 51.017 26.293 1.00 44.01 ATOM 8177 CG2 VAL E 376 48.960 50.549 24.615 1.00 41.99 C ATOM 8178 N HISE 377 48.120 47.391 27.711 1.00 43.66 N ATOM 8179 CA HIS E 377 47.416 46.562 28.698 1.00 44.10 C C ATOM 8180 C HIS E 377 48.161 46.583 30.004 1.00 43.06 ATOM 8181 O HISE 377 47.596 47.052 30.994 1.00 43.74 0 47.186 45.144 28.150 1.00 45.65 C ATOM 8182 CB HISE 377 ATOM 8183 CG AHIS E 377 46.526 44.179 29.078 0.50 44.17 C C ATOM 8184 CG BHIS E 377 46.100 45.198 27.098 0.50 48.43 ATOM 8185 ND1AHIS E 377 45.200 44.280 29.448 0.50 43.92 N ATOM 8186 ND1BHIS E 377 46.290 44.797 25.788 0.50 48.69 N ATOM 8187 CD2AHIS E 377 47.005 43.091 29.723 0.50 44.07 C C ATOM 8188 CD2BHIS E 377 44.810 45.630 27.175 0.50 49.00 C ATOM 8189 CE1AHIS E 377 44.898 43.302 30.282 0.50 43.39

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		CD1 TRP E 383		
ATOM	8236	CD2 TRP E 383	45.753 54.280 36.919 1.00 38.22	C
ATOM	8237	NEI TRP E 383	44.154 52.898 36.133 1.00 37.35	N
ATOM	8238	CE2 TRP E 383	44.361 54.007 36.924 1.00 38.41	C
			46.244 55.367 37.659 1.00 37.25	
ATOM	8240	CZ2 TRP E 383	43.472 54.816 37.635 1.00 37.58	C
ATOM	8241	CZ3 TRP E 383	45.347 56.146 38.354 1.00 36.24	C
ATOM	8242	CH2 TRP E 383	43.979 55.875 38.321 1.00 36.44	C
ATOM	8243	N LEU E 384	47.314 52.548 38.843 1.00 37.45	N
ATOM	8244	CA LEUE 384	47.090 52.912 40.242 1.00 35.59	
ATOM	8245	C LEU E 384	47.983 52.128 41.184 1.00 35.15	C
ATOM	8246	O LEU E 384	48.381 52.659 42.213 1.00 33.91	0_
ATOM	8247	CB LEUE 384	45.600 52.817 40.542 1.00 34.80	C
ATOM	8248	CG LEUE 384	45.114 53.321 41.892 1.00 35.29	C
ATOM	8249	CD1 LEU E 384	45.618 54.739 42.208 1.00 35.78	C
ATOM	8250	CD2 LEU E 384	43.596 53.340 41.977 1.00 33.47	C
			48.354 50.871 40.891 1.00 36.22	N
			49.202 50.124 41.837 1.00 35.99	
ATOM	8253	C GLU E 385	50.530 50.872 41.839 1.00 35.17	С
ATOM	8254	O GLUE 385	51.029 51.208 42.902 1.00 34.47	0
			49.349 48.648 41.567 1.00 36.38	
ATOM	8256	CG GLUE 385	48.330 47.663 42.046 1.00 37.25	С
ATOM	8257	CD GLUE 385	48.535 46.270 41.481 1.00 39.83	С
ATOM	8258	OE1 GLUE 385	48.115 46.085 40.310 1.00 39.19	0
			49.090 45.352 42.167 1.00 42.19	0
			51.042 51.136 40.638 1.00 35.91	
ATOM	8261	CA ILE E 386	52.295 51.859 40.493 1.00 36.84	С
ATOM	8262	C ILE E 386	52.198 53.189 41.248 1.00 37.39	
ATOM	8263	O ILE E 386	53.101 53.418 42.031 1.00 37.87	0
			52.733 52.263 39.081 1.00 37.29	
ATOM	8265	CG1 ILE E 386	52.655 51.193 38.000 1.00 39.11	
ATOM	8266	CG2 ILE E 386	54.153 52.766 39.108 1.00 36.98	С
		CD1 ILE E 386	53.450 49.952 38.250 1.00 40.93	С
ATOM	8268	N LEU E 387	51.181 54.024 41.039 1.00 37.44	N
		CA LEUE 387	51.079 55.276 41.749 1.00 36.84	C
		C LEU E 387	51.104 55.057 43.250 1.00 37.11	С
ATOM	8271	O LEU E 387	51.809 55.773 43.946 1.00 37.83	0
ATOM	8272	CB LEUE 387	49.787 56.045 41.473 1.00 37.36	C
ATOM	8273	CG LEUE 387	49.672 56.828 40.166 1.00 38.07	C
ATOM	8274	CD1 LEU E 387	48.281 57.449 40.044 1.00 37.57	С
ATOM	8275	CD2 LEU E 387	50.758 57.878 40.028 1.00 37.61	С
ATOM	8276	N MET E 388	50.345 54.083 43.735 1.00 37.87	N
ATOM	8277	CA MET E 388	50.270 53.824 45.165 1.00 37.01	С
ATOM	8278	C MET E 388	51.599 53.354 45.697 1.00 37.19	С
ATOM	8279	O MET E 388	51.935 53.886 46.766 1.00 38.13	0

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A TON	8280 CB MET E 388	49.170 52.880 45.613 1.00 36.22	C ·
ATOM	9291 CG MET E 388	47.791 53.146 45.057 1.00 37.20	
ATOM	9292 SD MET E 388	46.461 52.382 45.966 1.00 39.84	S
ATOM	8283 CF MET F 388	44.984 53.248 45.589 1.00 38.34	
	8284 N ILE E 389		N
		53.616 52.093 45.726 1.00 39.29	C
ATOM	2285 CA IEEE 380	54.578 53.267 45.831 1.00 40.45	C
ATOM	8287 O HEF 389	55.356 53.490 46.761 1.00 40.75	Ö
		54.222 50.827 45.123 1.00 37.83	C
ATOM	8280 CGI II F F 389	55.425 50.346 45.924 1.00 36.80	C
ATOM	8200 CG2 II E E 380	54 505 51 106 43 602 1 00 37 39	Č
ATOM	8290 CO2 ILE E 389	54.595 51.106 43.692 1.00 37.39 55.773 48.905 45.705 1.00 35.84	Č
ATOM	9291 CDI ILE E 389	54.524 54.172 44.875 1.00 41.61	
		55.351 55.364 44.814 1.00 41.77	
		55.025 56.190 46.034 1.00 41.56	c
		55.923 56.518 46.787 1.00 42.11	Ö
ATOM	8295 O GETE 390	53.738 56.469 46.198 1.00 41.60	N
ATOM	8290 N LEUE 391	53.307 57.279 47.342 1.00 41.33	Ċ
ATOM	9297 CA LLU L 391	53.820 56.698 48.639 1.00 41.79	c
ATOM	8290 O IEIIE 301	54.482 57.320 49.453 1.00 41.82	Ö .
ATOM	8300 CR LEVE 391	51.786 57.333 47.403 1.00 41.22	C
		51.154 57.962 48.635 1.00 41.26	
ATOM	8302 CD1 LEUE 391	51.615 59.406 48.746 1.00 41.59	
ATOM	8303 CD2 I FILE 391	49.649 57.899 48.614 1.00 41.44	Ċ
		53.493 55.428 48.846 1.00 42.92	N
		53.904 54.714 50.049 1.00 43.47	C
ATOM	8306 C VALE 392	55.391 54.884 50.312 1.00 43.90	
ATOM	8307 O VALE 392	55.872 55.202 51.385 1.00 43.97	0
ATOM	8308 CB VALE 392	53.514 53.225 49.916 1.00 42.03	C
ATOM	8309 CGI VALE 392	54.100 52.390 51.034 1.00 42.06	С
ATOM	8310 CG2 VAL E 392	52.006 53.137 50.059 1.00 42.59	· C
	8311 N TRP E 393	56.176 54.635 49.285 1.00 45.06	N
	8312 CA TRP E 393	57.617 54.695 49.353 1.00 46.99	C
	8313 C TRP E 393	58.092 56.087 49.703 1.00 48.48	С
	8314 O TRP E 393	58,947 56,258 50,563 1,00 50,59	0
	8315 CB TRP E 393	58.184 54.330 47.988 1.00 47.26	C
	8316 CG TRP E 393	59.584 54.800 47.814 1.00 47.60	C
	8317 CD1 TRP E 393	60,002 55.829 47.036 1.00 48.13	C
	8318 CD2 TRP E 393	60.749 54.273 48.451 1.00 48.09	С
	8319 NE1 TRP E 393	61.371 55.962 47.135 1.00 48.58	N
	8320 CE2 TRP E 393	61.854 55.011 47.991 1.00 47.67	С
	8321 CE3 TRP E 393	60.969 53.232 49.357 1.00 48.54	С
	8322 CZ2 TRP E 393		С
	8323 CZ3 TRP E 393		С
	8324 CH2 TRP E 393	63.315 53.732 49.268 1.00 47.93	С

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C

49.276 62.739 47.924 1.00 45.05

48.843 62.814 49.221 1.00 45.82

48.777 61.777 47.084 1.00 44.28

47.889 61.924 49.695 1.00 46.11 47.838 60.888 47.541 1.00 44.40

ATOM 8410 CG PHE E 404

ATOM 8411 CD1 PHE E 404

ATOM 8412 CD2 PHE E 404

ATOM 8413 CE1 PHE E 404

ATOM 8414 CE2 PHE E 404

			2 -01	
			47.400 60.966 48.842 1.00 45.60	
ATOM	8416	N ALA E 405	53.213 64.996 47.448 1.00 49.95	N
ATOM	8417	CA ALA E 405	54.261 65.757 46.787 1.00 52.59	С
ATOM	8418	C ALA E 405	55.197 66.307 47.835 1.00 53.64	С
ATOM	8419	O ALA E 405	54.871 66.317 49.018 1.00 55.50	0
ATOM	8420	CB ALA E 405	53.650 66.938 46.034 1.00 53.32	С
ATOM	8421	N PRO E 406	56.315 66.857 47.408 1.00 54.23	N
ATOM	8422	CA PRO E 406	57.308 67.482 48.284 1.00 54.34	С
ATOM	8423	C PRO E 406	56.574 68.626 48.967 1.00 54.49	С
ATOM	8424	O PRO E 406	56.811 68.813 50.148 1.00 56.57	0
ATOM	8425	CB PRO E 406	58.508 67.936 47.470 1.00 53.22	С
ATOM	8426	CG PRO E 406 -	58.228 67.270 46.164 1.00 53.88	С
ATOM	8427	CD PRO E 406	56.744 66.938 46.023 1.00 54.30	С
ATOM	8428	N ASN E 407	55.682 69.300 48.272 1.00 53.76	N
ATOM	8429	CA ASN E 407	54.909 70.361 48.867 1.00 54.30	С
ATOM	8430	C ASN E 407	53.465 69.995 49.121 1.00 55.11	С
ATOM	8431	O ASN E 407	52.622 70.904 49.123 1.00 56.53	Ο
			55.011 71.560 47.924 1.00 55.00	С
ATOM	8433	CG ASN E 407	54.181 71.361 46.688 1.00 55.76	С
ATOM	8434	OD1 ASN E 407	54.138 70.284 46.113 1.00 57.06	0
			53.492 72.405 46.279 1.00 57.34	N
			53.107 68.731 49.307 1.00 55.09	N
ATOM	8437	CA LEU E 408	51.700 68.394 49.595 1.00 54.77	
		C LEU E 408		C
ATOM			52.083 66.123 50.085 1.00 56.28	0
ATOM			50.797 68.071 48.453 1.00 53.54	С
ATOM	8441		49.357 67.658 48.721 1.00 52.83	С
ATOM	8442	CD1 LEU E 408	48.613 68.523 49.692 1.00 51.64	С
			48.579 67.655 47.396 1.00 53.46	C
			51.637 67.479 51.860 1.00 56.09	N
			51.790 66.390 52.829 1.00 55.60	C
ATOM	8446	C LEU E 409	50.546 66.225 53.671 1.00 55.76	С
ATOM		O LEU E 409	50.441 66.799 54.737 1.00 56.37	Ο
		CB LEU E 409	53.027 66.737 53.616 1.00 55.29	С
		CG LEU E 409	53.557 65.981 54.811 1.00 54.70	С
		CD1 LEU E 409	53.370 64.493 54.726 1.00 54.26	С
		CD2 LEU E 409	55.061 66.263 54.928 1.00 55.29	С
		N LEUE 410	49.574 65.443 53.205 1.00 56.47	N
		CA LEUE 410	48.342 65.262 53.952 1.00 56.35	С
		C LEUE 410	48.637 64.342 55.114 1.00 58.87	C
		O LEU E 410	49.603 63.582 55.135 1.00 59.73	0
		CB LEUE 410	47.193 64.774 53.099 1.00 54.74	C
		CG LEUE 410	47.035 65.606 51.825 1.00 54.12	С
		CD1 LEU E 410	45.915 65.082 50.962 1.00 54.60	C
ATOM	8459	CD2 LEU E 410	46.804 67.054 52.215 1.00 53.95	С

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ATOM	8505 CG LYS E 416	38.708 62.042 58.641 1.00 74.66	С
ATOM	8506 CD LYS E 416	37.872 61.379 59.724 1.00 77.68 38.165 61.959 61.103 1.00 80.25	С
ATOM	8507 CE LYS E 416	38.165 61.959 61.103 1.00 80.25	C
ATOM	8508 NZ LYS E 416	39.365 61.334 61.753 1.00 82.62	N
ATOM	8509 N CYS E 417	38.193 64.535 54.744 1.00 67.34	
		37.629 65.560 53.895 1.00 67.24	C
		36.866 64.908 52.769 1.00 65.36	C
		35.771 65.380 52.469 1.00 66.59	0
ATOM	8513 CB CYSE 417	38.722 66.539 53.457 1.00 69.38 39.355 67.479 54.900 1.00 74.04	C S
ATOM	0515 N VAI E 417	37.350 63.853 52.141 1.00 63.31	
ATOM	8516 CA VALE 418	36.658 63.184 51.054 1.00 60.57	
ATOM	8517 C VALE 418	35 994 61 907 51 541 1.00 60 34	c
ATOM	8518 O VAL E 418	35.994 61.907 51.541 1.00 60.34 36.608 61.182 52.293 1.00 59.16	Ö
ATOM	8519 CB VALE 418	37.604 62.859 49.901 1.00 59.16	C
		36.927 62.062 48.805 1.00 58.97	С
ATOM	8521 CG2 VAL E 418	38.147 64.151 49.318 1.00 58.63	C
ATOM	8522 N GLU E 419	34.773 61.664 51.136 1.00 62.30	N
		33.967 60.513 51.471 1.00 65.39	С
ATOM	8524 C GLUE 419	34.668 59.207 51.171 1.00 64.79	С
ATOM	8525 O GLUE 419	35.275 58.988 50.122 1.00 65.46	0
ATOM	8526 CB GLUE 419	32.700 60.554 50.628 1.00 70.25	C
		31.397 60.207 51.316 1.00 76.71	
		30.289 59.850 50.330 1.00 80.65 30.259 60.410 49.200 1.00 82.59	
ATOM	8529 OE1 GLU E 419	29.420 58.996 50.660 1.00 82.71	0
		34.663 58.263 52.095 1.00 63.96	N
		35.329 57.000 51.876 1.00 63.44	
		36.825 56.991 51.685 1.00 62.43	
ATOM	8534 O GLY E 420	37.362 55.901 51.460 1.00 63.54	О
	8535 N MET E 421	37.589 58.040 51.788 1.00 61.69	N
	8536 CA MET E 421	39.015 58.104 51.653 1.00 61.14	С
	8537 C MET E 421		С
		41.021 57.282 52.649 1.00 60.75	0
	8539 CB MET E 421	39.400 59.586 51.439 1.00 62.19	C
	8540 CG MET E 421	39.464 59.848 49.952 1.00 63.76	C
	8541 SD MET E 421	41.214 59.747 49.509 1.00 64.70	S C
	8542 CE MET E 421 8543 N VAL E 422	41.583 61.487 49.813 1.00 65.67 39.411 57.829 54.048 1.00 60.12	N
	8544 CA VALE 422	40.143 57.500 55.249 1.00 59.26	C
	8545 C VALE 422	40.593 56.051 55.239 1.00 58.74	c
	8546 O VALE 422	41.732 55.886 55.666 1.00 58.75	Ö
	8547 CB VALE 422	39.340 57.632 56.564 1.00 59.81	C
		40.170 58.363 57.610 1.00 60.12	C
		38.025 58.347 56.309 1.00 60.75	С

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ATOM	8550 N GLUE 423	39.739 55.125 54.804 1.00 57.81	N
ATOM	8551 CA GLUE 423	40.127 53.727 54.792 1.00 58.23	С
ATOM	8552 C GLU E 423	41.281 53.498 53.819 1.00 55.38	С
		42.217 52.767 54.120 1.00 54.90	0
ATOM	8554 CB GLUE 423	39.014 52.779 54.396 1.00 63.04	C
ATOM	8555 CG GLUE 423	37.777 52.932 55.260 1.00 69.79	C
ATOM	8556 CD GLUE 423	36.871 54.029 54.697 1.00 74.22	C
ATOM	8557 OE1 GLU E 423	37.159 55.247 54.849 1.00 74.78	O O
		35.839 53.636 54.066 1.00 77.24	N
ATOM	8339 N ILEE 424	41.175 54.147 52.664 1.00 51.41 42.266 54.040 51.697 1.00 47.98	C
		43.493 54.655 52.339 1.00 48.22	Č ;
ATOM	8562 O T.E.E.424	44.569 54.017 52.381 1.00 49.81	Ö
ΔΤΟΜ	8563 CB TLE E 424	41.809 54.691 50.412 1.00 46.43	C
ATOM	8564 CG1 ILE E 424	40.626 53.844 49.916 1.00 45.58	С
ATOM	8565 CG2 ILE E 424	40.626 53.844 49.916 1.00 45.58 42.919 54.746 49.387 1.00 46.53	С
ATOM	8566 CD1 ILE E 424	39.973 54.492 48.721 1.00 45.49	С
ATOM	8567 N PHE E 425	43.404 55.835 52,944 1.00 46.64	N
ATOM	8568 CA PHE E 425	44.559 56.416 53.614 1.00 46.97	
	8569 C PHE E 425		С
ATOM	8570 O PHE E 425	46.309 55.306 54.875 1.00 48.59	0
ATOM	8571 CB PHE E 425	44.198 57.739 54.285 1.00 46.71	C
ATOM	8572 CG PHE E 425	44.315 58.934 53.392 1.00 46.51	C
ATOM	8573 CD1 PHE E 425	44.121 58.804 52.022 1.00 47.41	C C
ATOM	8574 CD2 PHE E 425	44.606 60.166 53.908 1.00 45.89	
ATOM	8575 CEI PHE E 425	44.226 59.870 51.169 1.00 47.79 44.713 61.243 53.061 1.00 47.82	
ATOM	85/0 CEZ PRE E 425	44.533 61.114 51.689 1.00 48.33	č
	8578 N ASP E 426		
		44.641 53.882 56.435 1.00 50.32	C
	8580 C ASP E 426		
	8581 O ASP E 426	46,560 52,514 56,382 1.00 50.94	O ·
	8582 CB ASP E 426	43,444 53,475 57,263 1.00 52.85	С
	8583 CG ASP E 426	43.164 54.520 58.338 1.00 55.13	С
	8584 OD1 ASP E 426	44.105 55.313 58.581 1.00 56.03	0
ATOM	8585 OD2 ASP E 426	42.050 54.547 58.918 1.00 55.96	0
	8586 N MET E 427	45.012 52.091 54.829 1.00 48.06	N
	8587 CA MET E 427	45.745 51.025 54.169 1.00 45.93	C
	8588 C MET E 427	47.068 51.572 53.631 1.00 44.99	C
	8589 O MET E 427	48.142 50.951 53.764 1.00 44.81	0
	8590 CB MET E 427	44.866 50.475 53.055 1.00 46.28	C C
	8591 CG MET E 427	43.702 49.673 53.618 1.00 47.12	S
	8592 SD MET E 427		C
	8593 CE MET E 427 8594 N LEU E 428	47.014 52.774 53.049 1.00 42.52	N
AIOM	0374 N LEUE 428	T1.017 J2.114 JJ.047 1.00 72.J2	**

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АТОМ	8595 CA LEUE 428	48.268 53.339 52.557 1.00 41.97	С
ATOM	8596 C LEUE 428	49.234 53.533 53.710 1.00 42.31	C
ATOM	8597 O LEU E 428	50.398 53.126 53.571 1.00 43.27	0
ATOM	8598 CB LEU E 428	48.026 54.630 51.795 1.00 41.62	С
ATOM	8599 CG LEUE 428	47.304 54.478 50.452 1.00 40.23 46.808 55.825 49.983 1.00 39.61	С
ATOM	8600 CD1 LEU E 428	46.808 55.825 49.983 1.00 39.61	С
ATOM	8601 CD2 LEU E 428	48.271 53.875 49.453 1.00 40.11	С
ATOM	8602 N LEUE 429	48.784 54.097 54.832 1.00 42.32	N
ATOM	8603 CA LEUE 429	49.695 54.316 55.966 1.00 42.13 50.303 53.027 56.474 1.00 41.73	C
ATOM	8604 C LEUE 429	50.303 53.027 56.474 1.00 41.73	C
ATOM	8605 O LEUE 429	51.522 52.889 56.618 1.00 42.13	0
ATOM	8606 CB LEU E 429	48.997 55.122 57.050 1.00 42.21	C
ATOM	8607 CG LEUE 429	48.743 56.587 56.666 1.00 42.47 47.706 57.199 57.578 1.00 42.17	C
ATOM	8608 CD1 LEU E 429	47.706 57.199 57.578 1.00 42.17	C C
ATOM	8609 CD2 LEU E 429	50.006 57.426 56.642 1.00 42.12	
ATOM	8610 N ALAE 430	49.476 52.023 56.684 1.00 41.47 49.927 50.709 57.111 1.00 42.24	C
ATOM	8011 CA ALAE 430	51.002 50.130 56.196 1.00 43.35	c
ATOM	8612 C ALA E 430	51.941 49.496 56.695 1.00 43.89	0
		48.738 49.757 57.062 1.00 42.20	
ATOM	8615 N THR F 431	50.863 50.314 54.877 1.00 42.68	
ATOM	8616 CA THR F 431	51.886 49.788 53.990 1.00 42.40	C
		53.149 50.600 54.194 1.00 43.01	C
		54.267 50.100 54.270 1.00 42.66	0
ATOM	8619 CB THR E 431	51.500 49.991 52.523 1.00 42.40	С
ATOM	8620 OG1 THR E 431	50.165 49.495 52.408 1.00 43.64	0
ATOM	8621 CG2 THR E 431	52.445 49.277 51.594 1.00 42.04	С
ATOM	8622 N SER E 432	52.895 51.914 54.285 1.00 44.22	N
ATOM	8623 CA SER E 432	54.030 52.832 54.444 1.00 45.72	C
ATOM	8624 C SER E 432	54.857 52.445 55.656 1.00 45.62	C
	8625 O SER E 432		0
		53,569 54.272 54.448 1.00 45.63	C
		54.753 55.052 54.544 1.00 46.77	0
	8628 N SER E 433		N
	8629 CA SER E 433	54.705 51.722 57.965 1.00 49.92	C
	8630 C SER E 433	55.450 50.400 57.864 1.00 50.55 56.573 50.223 58.340 1.00 50.04	C O
	8631 O SER E 433 8632 CB SER E 433	53,466 51.523 58.844 1.00 52.38	C
	8633 OG SER E 433	53.946 51.508 60.181 1.00 56.50	O
	8634 N ARGE 434	54.867 49.401 57.191 1.00 51.62	N
		55.543 48.117 57.014 1.00 52.03	C
	8636 C ARGE 434	56.826 48.346 56.234 1.00 52.24	C
	8637 O ARGE 434	57.810 47.709 56.557 1.00 51.44	Ō
	8638 CB ARG E 434	54.666 47.066 56.355 1.00 53.23	С
		55.424 45.815 55.995 1.00 56.12	С

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ATOM	8640 CD ARG E 434	54,742 44,525 56,408 1.00 59.27	С
ATOM	8641 NE ARG E 434	55.682 43.366 56.334 1.00 60.61 56.551 43.176 57.327 1.00 60.77	N
ATOM	8642 CZ ARG E 434	56.551 43.176 57.327 1.00 60.77	С
ATOM	8643 NH1 ARG E 434	56.504 44.063 58.319 1.00 61.70	N
ATOM	8644 NH2 ARG E 434	57.407 42.174 57.336 1.00 61.04	N
ATOM	8645 N PHE E 435	56.857 49.236 55.241 1.00 53.65	N
ATOM	8646 CA PHE E 435	58.075 49.492 54.496 1.00 55.21	C
		59.110 50.101 55.429 1.00 57.28	С
ATOM	8648 O PHE E 435	60.298 49.827 55.313 1.00 56.92	0
ATOM	8649 CB PHE E 435	57.856 50.389 53.292 1.00 55.58	C
ATOM	8650 CG PHE E 435	57.856 50.389 53.292 1.00 55.58 57.346 49.723 52.044 1.00 55.83	С
ATOM	8651 CD1 PHE E 435	57.272 48.349 51.909 1.00 55.27	C .
ATOM	8652 CD2 PHE E 435	56.921 50.492 50.970 1.00 55.48	С
ATOM	8653 CE1 PHE E 435	56.791 47.753 50.771 1.00 54.62	С
ATOM	8654 CE2 PHE E 435	56.435 49.929 49.819 1.00 54.80	С
ATOM	8655 CZ PHE E 435	56.374 48.548 49.732 1.00 55.27	С
ATOM	8656 N ARG E 436	58.667 50.933 56.369 1.00 59.99	N
ATOM	8657 CA ARG E 436	59.564 51.547 57.333 1.00 62.20	С
ATOM	8658 C ARG E 436	60.182 50.457 58.189 1.00 62.86	С
ATOM	8659 O ARG E 436	61.371 50.353 58.390 1.00 62.51	
		58.806 52.531 58.210 1.00 63.59	
ATOM	8661 CG ARG E 436	59.645 53.678 58.742 1.00 66.33	С
ATOM	8662 CD ARG E 436	58.855 54.573 59.699 1.00 68.41 57.704 55.162 59.009 1.00 70.77	С
ATOM	8663 NE ARG E 436	57.704 55.162 59.009 1.00 70.77	N
ATOM	8664 CZ ARG E 436	56.438 54.917 59.357 1.00 71.97	С
ATOM	8665 NH1 ARG E 436	56.195 54.113 60.387 1.00 72.22	N
ATOM	8666 NH2 ARG E 436	55.429 55.469 58.682 1.00 72.49	N
ATOM	8667 N MET E 437	59.352 49.583 58.719 1.00 65.85	N
ATOM	8668 CA MET E 437	59.780 48.495 59.572 1.00 68.28	C
ATOM	8669 C MET E 437	60.781 47.598 58.902 1.00 66.41	С
		61.737 47.225 59.562 1.00 67.60	
		58.597 47.637 60.008 1.00 73.91	
	8672 CG MET E 437		C
	8673 SD MET E 437		S
	8674 CE MET E 437	55.761 46.302 60.604 1.00 84.74	C
	8675 N MET E 438	60.639 47.235 57.653 1.00 64.77	N
	8676 CA MET E 438	61.542 46.352 56.940 1.00 62.86	C
	8677 C MET E 438	62.758 47.063 56.394 1.00 62.06	С
	8678 O MET E 438	63.655 46.472 55.819 1.00 61.19	0
	8679 CB MET E 438	60.834 45.849 55.687 1.00 63.11	С
	8680 CG MET E 438	59.521 45.168 56.012 1.00 63.13	C
	8681 SD MET E 438		S C
		60.614 43.488 53.985 1.00 64.56	
	8683 N ASNE 439		N C
ATOM	8084 CA ASN E 439	63.787 49.228 56.103 1.00 64.19	C

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ATOM	8730 N PHE E 445	62.973 48.969 46.192 1.00 45.85	N
	8731 CA PHE E 445	61.777 49.707 45.775 1.00 44.80	С
ATOM	8732 C PHE E 445	61.576 49.615 44.275 1.00 45.78	С
ATOM	8733 O PHE E 445	60.573 49.140 43.752 1.00 46.63	Ο
ATOM	8734 CB PHE E 445	61.848 51.154 46.205 1.00 43.02	С
ATOM	8735 CG PHE E 445	60.831 52.044 45.569 1.00 43.23	С
ATOM	8736 CD1 PHE E 445	59.476 51.796 45.716 1.00 44.18	С
ATOM	8737 CD2 PHE E 445	61.198 53.137 44.817 1.00 43.23	С
ATOM	8738 CE1 PHE E 445	58.511 52.599 45.142 1.00 43.74	С
ATOM	8739 CE2 PHE E 445	60.260 53.959 44.224 1.00 43.01	С
ATOM	8740 CZ PHE E 445	58.924 53.684 44.396 1.00 43.58	С
ATOM	8741 N VAL E 446	62.579 50.068 43.545 1.00 46.16	N
ATOM	8742 CA VAL E 446	62.630 50.077 42.088 1.00 45.68	С
ATOM	8743 C VAL E 446	62.362 48.707 41.495 1.00 46.43	С
ATOM	8744 O VAL E 446	61.741 48.586 40.426 1.00 47.33	0
ATOM	8745 CB VAL E 446	63.991 50.727 41.796 1.00 45.32	С
ATOM	8746 CG1 VAL E 446	64.914 49.963 40.872 1.00 45.72	C
ATOM	8747 CG2 VAL E 446	63.724 52.122 41.284 1.00 45.43	C
ATOM	8748 N CYS E 447	62.769 47.617 42.126 1.00 45.86	N
ATOM	8749 CA CYS E 447	62.510 46.308 41.588 1.00 47.15	С
ATOM	8750 C CYS E 447	61.044 45.938 41.706 1.00 47.41	С
ATOM	8751 O CYS E 447	60.444 45.386 40.804 1.00 47.17	Ο
ATOM	8752 CB CYS E 447	63.340 45.289 42.408 1.00 48.11	С
ATOM	8753 SG CYS E 447	65.012 45.131 41.773 1.00 48.83	S
ATOM	8754 N LEUE 448	60.468 46.211 42.884 1.00 48.29	N
ATOM	8755 CA LEU E 448	59.075 45.863 43.186 1.00 46.52	С
ATOM	8756 C LEU E 448	58.158 46.558 42.207 1.00 44.79	С
ATOM	8757 O LEU E 448	57.273 45.984 41.603 1.00 45.09	О
ATOM	8758 CB LEU E 448	58.711 46.262 44.602 1.00 46.56	С
ATOM	8759 CG LEUE 448	59.263 45.396 45.726 1.00 47.45	С
ATOM	8760 CD1 LEU E 448	58.865 46.048 47.051 1.00 49.15	С
ATOM	8761 CD2 LEU E 448	58.698 43.984 45.668 1.00 47.57	С
ATOM	8762 N LYS E 449		N
ATOM	8763 CA LYS E 449	57.700 48.661 41.087 1.00 42.55	С
	8764 C LYS E 449	57.667 48.014 39.725 1.00 41.51	С
	8765 O LYS E 449	56.576 47.973 39.148 1.00 41.11	О
	8766 CB LYS E 449	58.259 50.070 41.163 1.00 43.23	С
	8767 CG LYS E 449	57.213 51.131 40.878 1.00 44.11	С
	8768 CD LYS E 449	57.814 52.207 40.038 1.00 45.17	С
	8769 CE LYS E 449	58.566 53.240 40.879 1.00 46.14	С
	8770 NZ LYS E 449	58.905 54.311 39.862 1.00 47.75	N
	8771 N SER E 450	58.762 47.480 39.200 1.00 41.28	N
	8772 CA SER E 450	58.747 46.784 37.917 1.00 41.19	C
	8773 C SER E 450	58.009 45.447 37.965 1.00 39.26	C
ATOM	8774 O SER E 450	57.345 45.088 37.013 1.00 38.89	О

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ATOM	8775 CB SER E 450	60.151 46.414 37.429 1.00 41.77	С
		60.812 47.665 37.489 1.00 45.16	
		58.116 44.741 39.066 1.00 37.81	
ATOM	8778 CA ILE E 451	57.411 43.491 39.217 1.00 38.28	С
		55.942 43.845 39.068 1.00 38.66	
ATOM	8780 O ILE E 451	55.260 43.153 38.304 1.00 39.09	0
ATOM	8781 CB ILE E 451	57.677 42.804 40.566 1.00 39.44	С
		59.159 42.383 40.551 1.00 40.75	
ATOM	8783 CG2 ILE E 451	56.735 41.649 40.826 1,00 36.95	С
ATOM	8784 CD1 ILE E 451	59.537 41.446 41.683 1.00 42.44 55.482 44.895 39.773 1.00 38.03	С
ATOM	8785 N ILE E 452	55.482 44.895 39.773 1.00 38.03	N
		54.077 45.292 39.670 1.00 36.73	
		53.667 45.590 38.228 1.00 37.55	
		52.630 45.154 37.740 1.00 37.79	
		53.778 46.525 40.539 1.00 35.25	
ATOM	8790 CG1 ILE E 452	54.042 46.194 41.990 1.00 34.33	C
ATOM	8791 CG2 ILE E 452	52.343 46.998 40.308 1.00 35.46 53.496 47.137 43.035 1.00 33.49	C
ATOM	8792 CD1 ILE E 452	53.496 47.137 43.035 1.00 33.49	C
		54.469 46.343 37.480 1.00 37.40	
		54.144 46.673 36.120 1.00 37.51	
ATOM	8795 C LEU E 453	54.016 45.399 35.317 1.00 39.84	
		53.143 45.302 34.468 1.00 41.15	0
		55.216 47.577 35.480 1.00 36.14	
		55.078 47.731 33.950 1.00 34.66	
ATOM	8/99 CD1 LEU E 453	53.789 48.461 33.614 1.00 33.30 56.293 48.419 33.373 1.00 33.44	C C
		54.913 44.438 35.483 1.00 42.17	
		54.884 43.238 34.678 1.00 43.70	
		53.940 42.135 35.110 1.00 44.73	
		53.478 41.386 34.231 1.00 45.81	
ATOM	8805 CR IFILE 454	56.313 42.619 34.636 1.00 43.59	C
ATOM	8806 CG LEUE 454	57.256 43.422 33.739 1.00 44.11	Č
	8807 CD1 LEU E 454	58.696 43.048 34.044 1.00 44.82	Č
	8808 CD2 LEU E 454	56.946 43.117 32.280 1.00 44.72	Č
	8809 N ASNE 455	53.681 41.966 36.397 1.00 44.67	N
	8810 CA ASN E 455	52.869 40.827 36.797 1.00 45.18	C
	8811 C ASN E 455	51.424 41.141 36.932 1.00 47.23	C
	8812 O ASN E 455	50.636 40.216 36.942 1.00 48.88	Ö
	8813 CB ASN E 455	53.419 40.284 38.114 1.00 45.05	C
	8814 CG ASN E 455	52.544 39.391 38.943 1.00 44.88	C
	8815 OD1 ASN E 455	51.977 39.852 39.945 1.00 44.69	O
	8816 ND2 ASN E 455	52.423 38.128 38.532 1.00 45.24	N
	8817 N SER E 456	51.007 42.368 37.060 1.00 51.07	N
	8818 CA SER E 456	49.584 42.600 37.276 1.00 54.67	С
ATOM	8819 C SER E 456	48.726 42.201 36.124 1.00 57.34	· C

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ATOM	8820 O SER E 456	47.729 41.484 36.251 1.00 60.01	0
ATOM	8821 CB SER E 456	49.364 44.032 37.754 1.00 55.11	C
ATOM	8822 OG SER E 456	49.674 44.134 39.133 1.00 54.61	0
ATOM	8823 N GLYE 457	49.004 42.608 34.919 1.00 60.38	N
ATOM	8824 CA GLY E 457	48.129 42.260 33.798 1.00 64.14	С
ATOM	8825 C GLY E 457	48.515 41.006 33.045 1.00 65.86	С
ATOM	8826 O GLY E 457	47.944 40.834 31.957 1.00 65.56	O
ATOM	8827 N VALE 458	49.425 40.210 33.596 1.00 67.97	N
ATOM	8828 CA VAL E 458	49.868 39.019 32.903 1.00 71.23	С
ATOM	8829 C VALE 458	48.824 37.951 32.696 1.00 74.98	С
ATOM	8830 O VALE 458	48.846 37.316 31.620 1.00 76.05	0
	8831 CB VAL E 458		C
		51.000 37.726 34.770 1.00 68.98	C
ATOM	8833 CG2 VAL E 458	51.843 37.570 32.447 1.00 70.96	С
ATOM	8834 N TYR E 459	47.851 37.716 33.554 1.00 79.48	N
ATOM	8835 CA TYR E 459	46.801 36.725 33.382 1.00 84.01	С
ATOM	8836 C TYR E 459		C
ATOM	8837 O TYR E 459	· · · · · · · · · · · · · · · · · · ·	0
ATOM	8838 CB TYR E 459		C
ATOM	8839 CG TYR E 459		C
ATOM		48.111 36.698 36.204 1.00 89.50	C
ATOM	8841 CD2 TYR E 459	47.823 34.424 35.638 1.00 89.47	C
ATOM		49.219 36.275 36.876 1.00 90.68	C
ATOM	8843 CE2 TYR E 459		C
ATOM	8844 CZ TYR E 459		C
ATOM		50.804 34.835 37.811 1.00 91.35	0
ATOM		45.816 38.308 31.793 1.00 88.41	N
ATOM		44.735 38.894 31.022 1.00 91.17	C
ATOM	8848 C THR E 460	45.242 39.429 29.693 1.00 92.86	C
		44.875 40.522 29.247 1.00 93.81	O C
	8850 CB THR E 460		. 0
ATOM		44.688 40.271 33.075 1.00 92.02	C
	8852 CG2 THR E 460	42.622 39.640 32.135 1.00 91.98	N
	8853 N PHE E 461	46.098 38.646 29.038 1.00 94.55	C
	8854 CA PHE E 461	46.656 39.112 27.775 1.00 95.80	C
	8855 C PHE E 461	45.738 39.274 26.580 1.00 97.31	0
	8856 O PHE E 461	45.871 40.307 25.864 1.00 98.52	C
	8857 CB PHE E 461	47.952 38.328 27.466 1.00 94.82	Ċ
	8858 CG PHE E 461	49.092 39.224 27.891 1.00 94.07	C
	8859 CD1 PHE E 461	48.944 40.596 27.851 1.00 94.00	C
	8860 CD2 PHE E 461	50.285 38.714 28.324 1.00 94.41	C
ATOM	8861 CE1 PHE E 461	49.941 41.453 28.227 1.00 94.40	C
ATOM	8862 CE2 PHE E 461	51.310 39.562 28.702 1.00 94.59	c
		51.145 40.931 28.653 1.00 94.60 46.792 34.388 20.855 1.00127.98	N
ATOM	8864 N THR E 465	40.792 34.388 20.833 1.00127.98	14

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ATOM	8865 CA THR E 465	47.001 33.276 21.784 1.00127.92	С
ATOM	8866 C THR E 465	47.001 33.276 21.784 1.00127.92 48.437 32.771 21.760 1.00126.90	С
ATOM	8867 O THR E 465	49.171 32.986 22.734 1.00127.57	0
ATOM	8868 CB THR E 465	46.057 32.091 21.526 1.00128.62	C
ATOM	8869 OG1 THR E 465	46.652 30.878 22.015 1.00128.85 45.724 31.947 20.051 1.00129.15	0
ATOM	8870 CG2 THR E 465	45.724 31.947 20.051 1.00129.15	С
ATOM	8871 N LEUE 466	48.894 32.147 20.677 1.00124.80	N
ATOM	8872 CA LEU E 466	50.282 31.668 20.608 1.00122.43	С
ATOM	8873 C LEUE 466	51.285 32.802 20.827 1.00120.18 52.355 32.585 21.413 1.00120.09	С
ATOM	8874 O LEUE 466	52.355 32.585 21.413 1.00120.09	Ο
		50.529 30.930 19.293 1.00122.67	
ATOM	8879 N LYSE 467	50.948 34.024 20.388 1.00116.78	N
ATOM	8880 CA LYS E 467	51.786 35.193 20.620 1.00113.09	С
		51.642 35.514 22.114 1.00109.31	
		52.603 35.953 22.740 1.00109.27	
ATOM	8883 CB LYS E 467	51.418 36.396 19.772 1.00114.44	C
ATOM	8884 CG LYS E 467	52.515 37.429 19.562 1.00115.60 51.923 38.725 19.019 1.00117.06	C C
ATOM	8883 CD LISE 407	52.004.28.020.17.522.1.00117.00	C
		52.094 38.930 17.523 1.00117.84 51.291 40.110 17.040 1.00117.85	
ATOM	9999 N CED E 469	50.467 35.264 22.689 1.00104.19	N
		50.220 35.488 24.095 1.00100.08	
ATOM	8890 C SFR F 468	51.034 34.533 24.965 1.00 96.75	c
		51.551 34.894 26.016 1.00 96.60	
ATOM	8892 CB SER E 468	48.758 35.266 24.491 1.00100.27	С
ATOM	8893 OG SER E 468	48.758 35.266 24.491 1.00100.27 47.938 36.279 23.954 1.00101.24	Ο
ATOM	8894 N LEU E 469	51.138 33.294 24.504 1.00 92.82	N
		51.890, 32.278 25.235 1.00 89.41	
ATOM	8896 C LEUE 469	53.354 32.681 25.198 1.00 87.00	С
ATOM	8897 O LEU E 469	54.092 32.455 26.147 1.00 86.58	O
		51.628 30.888 24.663 1.00 89.70	С
	8902 N GLUE 470	53.784 33.307 24.111 1.00 84.85	N
	8903 CA GLUE 470	55.169 33.762 23.995 1.00 83.18	C
	8904 C GLUE 470	55.307 35.050 24.783 1.00 78.98	C
	8905 O GLUE 470	56.319 35.293 25.418 1.00 78.25	0
	8906 CB GLUE 470	55.541 33.829 22.538 1.00 87.28	C
	8907 CG GLUE 470	56.196 35.110 22.067 1.00 93.08	C
	8908 CD GLUE 470	56.134 35.283 20.553 1.00 96.47	C O
	8909 OE1 GLU E 470 8910 OE2 GLU E 470	55.328 34.582 19.878 1.00 98.20 56.911 36.135 20.052 1.00 98.08	0
	8911 N GLUE 471	54.283 35.888 24.816 1.00 74.96	N
	8911 N GLUE 471 8912 CA GLUE 471	54.280 37.123 25.586 1.00 71.37	C
	8913 C GLUE 471	54.343 36.754 27.068 1.00 69.96	c
	8914 O GLUE 471	55.099 37.332 27.848 1.00 70.04	Ö
	8915 CB GLUE 471	53.037 37.965 25.326 1.00 69.94	C
, 11 OIVI	UNIO CE CEO E TITE	55,657 57,765 25,520 1.00 0 7.74	_

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ATOM	8961	ND1 HIS E 476	55.162 34.427 34.699 1.00 62.16 54.585 33.264 32.927 1.00 62.05 53.841 34.236 34.733 1.00 62.92	N
ATOM	8962	CD2 HIS E 476	54.585 33.264 32.927 1.00 62.05	С
ATOM	8963	CE1 HIS E 476	53.841 34.236 34.733 1.00 62.92	С
ATOM	8964	NE2 HIS E 476	53,456 33,533 33,678 1.00 62,30	N
ATOM	8965	N ARG E 477	59.914 35.209 32.362 1.00 57.98	N
ATOM	8966	CA ARGE 477	61.342 35.220 32.256 1.00 58.02	С
ATOM	8967	C ARG E 477	61.969 36.454 32.867 1.00 55.67	С
ATOM	8968	O ARGE 477	62.922 36.364 33.622 1.00 56.06	Ο
ATOM	8969	CB ARGE 477	61.713 35.226 30.771 1.00 62.72 62.916 34.325 30.544 1.00 68.93 62.323 32.907 30.431 1.00 74.07	С
ATOM	8970	CG ARGE 477	62,916 34,325 30,544 1,00 68,93	С
ATOM	8971	CD ARGE 477	62.323 32.907 30.431 1.00 74.07	С
ATOM	8972	NE ARGE 477	61.522 32.895 29.202 1.00 79.55	N
ATOM	8973	CZ ARGE 477	62.084 32.880 27.978 1.00 82.67 63.417 32.868 27.852 1.00 83.92	C
ATOM	8974	NH1 ARG E 477	63.417 32.868 27.852 1.00 83.92	N
ATOM	8975	NH2 ARG E 477	61.270 32.874 26.912 1.00 83.54	N
ATOM	8976	N VALE 478	61.457 37.628 32.539 1.00 53.33	N
ATOM	8977	CA VALE 478	61.979 38.885 33.065 1.00 51.57	С
ATOM	8978	C VALE 478	61.718 38.952 34.560 1.00 51.33	C
ATOM	8979	O VALE 478	62.521 39.436 35.371 1.00 50.99	O C
ATOM	8980	CB VALE 478	61.318 40.058 32.342 1.00 51.59	
ATOM	8981	CGI VALE 4/8	61.843 41.394 32.837 1.00 51.45 61.567 39.870 30.849 1.00 52.54	C
				N
ATOM	8983	N LEUE 4/9	60.546 38.412 34.941 1.00 49.88	
ATOM	8984	CA LEUE 479	60.155 38.337 36.338 1.00 48.08 61.167 37.502 37.124 1.00 49.08	
ATOM	8086	O LEUE 479	61.475 37.835 38.287 1.00 49.48	
ATOM	9097	CR I FILE 470	58.738 37.807 36.523 1.00 44.80	C
ATOM	8088	CG LEUE 479	57.638 38.850 36.416 1.00 43.44	
ATON (9090	CDIFFIE 470	56 280 28 165 36 412 1 00 43 41	C
ATOM	8990	CD2 LEUE 479	57.664 39.894 37.513 1.00 42.27	C
ATOM	8991	N ASP E 480	61.718 36.448 36.508 1.00 49.49	N
		CA ASP E 480	62.721 35.659 37.214 1.00 50.30	С
		C ASP E 480	63.993 36.490 37.309 1.00 50.24	С
			64.647 36.473 38.340 1.00 49.46	0
		CB ASP E 480	63.032 34.332 36.570 1.00 51.42	C
			61.883 33.364 36.553 1.00 53.00	С
			61.007 33.431 37.432 1.00 54.16	0
ATOM	8998	OD2 ASP E 480	61.807 32.498 35.653 1.00 54.42	Ο
ATOM	8999	N LYSE 481	64.294 37.214 36.236 1.00 51.72	N
ATOM	9000	CA LYS E 481	65.507 38.038 36.234 1.00 54.39	C
		C LYSE 481	65.403 39.049 37.363 1.00 52.96	С
		O LYS E 481	66.364 39.147 38.115 1.00 53.28	0
		CB LYSE 481	65.793 38.730 34.903 1.00 58.02	С
		CG LYS E 481	67.175 39.344 34.731 1.00 62.09	С
ATOM	9005	CD LYSE 481	68.162 38.389 34.087 1.00 65.98	С

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4 TO 1 4	0006	CE LYS E 481	69.605 38.540 34.546 1.00 69.03	С
ATOM ATOM		NZ LYS E 481	69,759 39,365 35,799 1.00 71.71	N
ATOM		N ILE E 482	64.252 39.720 37.470 1.00 51.11	N
ATOM		CA ILE E 482	64.085 40.703 38.535 1.00 48.85	С
ATOM		C ILE E 482	64.168 40.007 39.872 1.00 47.88	С
ATOM		O ILE E 482	64.789 40.547 40.798 1.00 47.61	0
ATOM	9012	CB ILE E 482	62.850 41.564 38.372 1.00 48.90	С
ATOM		CG1 ILE E 482	62.979 42.430 37.114 1.00 49.83	C
ATOM		CG2 ILE E 482	62.686 42.515 39.541 1.00 48.66	C
ATOM		CD1 ILE E 482	61.675 42.574 36.355 1.00 50.34	C
ATOM		N THRE 483	63.635 38.800 39.991 1.00 47.59	N
ATOM		CA THR E 483	63.789 38.092 41.270 1.00 49.09	C
ATOM		C THR E 483	65.261 37.914 41.614 1.00 50.39	C O
ATOM		O THR E 483	65.722 38.227 42.715 1.00 51.42 63.104 36.723 41.224 1.00 49.12	C
ATOM		CB THR E 483 OG1 THR E 483	61.695 36.995 41.063 1.00 50.26	o
ATOM ATOM		CG2 THR E 483	63.398 35.939 42.479 1.00 48.46	č
ATOM		N ASP E 484	66.058 37.432 40.643 1.00 50.79	N
ATOM		CA ASP E 484	67.484 37.245 40.832 1.00 49.22	C
ATOM		C ASP E 484	68.094 38.564 41.260 1.00 48.29	С
ATOM		O ASP E 484	68,896 38.610 42.191 1.00 49.77	0
ATOM		CB ASP E 484	68.170 36.726 39.587 1.00 50.22	C
ATOM		CG ASP E 484	67.746 35.330 39.199 1.00 51.85	С
ATOM	9029	OD1 ASP E 484	67.187 34.618 40.058 1.00 52.04	O
ATOM	9030	OD2 ASP E 484	67.976 34.955 38.012 1.00 53.07	0
ATOM		N THR E 485	67.724 39.671 40.648 1.00 47.30	N
ATOM		CA THR E 485	68.307 40.957 41.023 1.00 48.09	C
ATOM		C THR E 485	68.041 41.258 42.493 1.00 50.40	С
ATOM	9034		68.888 41.782 43.230 1.00 50.86	O C
		CB THR E 485	67.688 42.030 40.127 1.00 46.75 67.890 41.599 38.792 1.00 46.68	o
ATOM		OG1 THR E 485 CG2 THR E 485	68.324 43.380 40.335 1.00 46.98	Č
		N LEUE 486	66.818 40.925 42.940 1.00 50.66	N
		CA LEU E 486		C
		C LEUE 486	67.342 40.380 45.273 1.00 51.60	С
		O LEU E 486	67.909 40.953 46.218 1.00 52.24	0
		CB LEU E 486	64.991 40.763 44.550 1.00 47.97	С
ATOM	9043	CG LEU E 486		С
		CD1 LEU E 486		C
		CD2 LEU E 486		C
		N ILEE 487	67.454 39.076 45.010 1.00 52.13	N
		CA ILE E 487	68.281 38.236 45.869 1.00 53.81	C
ATOM	9048	C ILE E 487	69.715 38.753 45.883 1.00 55.54	C
			70.364 38.863 46.912 1.00 55.11	O C
ATOM	9050	CB ILE E 487	68.282 36.788 45.368 1.00 53.59	C

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ATOM	9145	CA GLN E 500	67 226 36 271 51 869 1 00 61 30	С
ATOM	9146	C GLN E 500	65.864 35.705 51.472 1.00 59.52 64.999 36.518 51.111 1.00 59.50	С
ATOM	9147	O GLN E 500	64.999 36.518 51.111 1.00 59.50	0
ATOM	9148	CB GLN E 500	68.304 35.728 50.970 1.00 62.53	С
ATOM	9149	CG GLN E 500	69.567 36.574 50.69 1.00 63.94	С
ATOM	9150	CD GLN E 500	70.657 35.694 50.265 1.00 64.75	С
ATOM	9151	OE1 GLN E 500	70.508 35.048 49.230 1.00 64.72	0
ATOM	9152	NE2 GLN E 500	71.778 35.663 50.965 1.00 66.02	N
ATOM	9153	N HISE 501	65.646 34.385 51.568 1.00 56.28 64.327 33.904 51.165 1.00 54.76 63.212 34.489 52.015 1.00 54.80	N
ATOM	9154	CA HIS E 501	64.327 33.904 51.165 1.00 54.76	С
ATOM	9155	C HIS E 501	63.212 34.489 52.015 1.00 54.80	С
ATOM	9156	O HIS E 501	62.118 34.664 51.456 1.00 56.59	O
ATOM	9157	CB HISE 501	64.183 32.405 51.063 1.00 54.63	С
ATOM	9158	CG AHIS E 501	64.301 31.550 52.271 0.50 53.86 65.370 31.733 50.443 0.50 55.35	С
ATOM	9159	CG BHIS E 501	65.370 31.733 50.443 0.50 55.35	С
ATOM	9160	ND1AHIS E 501	65.085 30.406 52.291 0.50 53.73	N
ATOM	9161	ND1BHIS E 501	65.831 32.076 49.196 0.50 55.39 63.744 31.631 53.495 0.50 53.43 66.186 30.756 50.904 0.50 55.24	N
ATOM	9162	CD2AHIS E 501	63.744 31.631 53.495 0.50 53.43	C
ATOM	9163	CD2BHIS E 501	66.186 30.756 50.904 0.50 55.24	C
ATOM	9164	CEIAHIS E 501	65.005 29.837 53.476 0.50 53.33	C
ATOM	9165	CE1BHIS E 501	66.886 31.338 48.908 0.50 55.63 64.196 30.564 54.223 0.50 53.32 67.120 30.534 49.931 0.50 55.54	С
ATOM	9166	NE2AHIS E 501	64.196 30.564 54.223 0.50 53.32	N
ATOM	9167	NE2BHIS E 501	67.120 30.534 49.931 0.50 55.54	N
ATOM	9168	N GLN E 502	63.388 34.815 53.283 1.00 52.93	N
ATOM	9169	CA GLN E 502	62.318 35.390 54.078 1.00 51.36 61.987 36.780 53.587 1.00 50.30 60.831 37.091 53.311 1.00 49.64	C
ATOM	9170	C GLN E 502	61.987 36.780 53.587 1.00 50.30	C
ATOM	9171	O GLN E 502	60.831 37.091 53.311 1.00 49.64	0
ATOM	9172	CB GLN E 502	62.717 35.357 55.551 1.00 52.69	C
ATOM	91/3	CD CINE 502	62.955 33.916 55.981 1.00 54.06	C
ATOM	9174	OFI GINE 502	62.980 33.648 57.462 1.00 54.41 63.315 34.510 58.275 1.00 55.01	0
ATOM	9175		62.628 32.406 57.783 1.00 54.39	
		N ARGE 503	62.974 37.649 53.412 1.00 49.44	N
		CA ARGE 503	62.730 38.998 52.915 1.00 47.48	C
		C ARGE 503	62.002 38.993 51.577 1.00 47.83	c
		O ARG E 503	61.044 39.720 51.335 1.00 48.42	Ö
		CB ARGE 503	64.039 39.753 52.713 1.00 45.77	C
		CG ARGE 503	63.784 41.259 52.699 1.00 45.18	Č
		CD ARGE 503	65.074 42.045 52.865 1.00 44.12	Č
		NE ARGE 503	64.912 43.436 52.480 1.00 43.85	N
		CZ ARGE 503	64.532 44.405 53.307 1.00 44.09	C
		NH1 ARG E 503	64.267 44.119 54.575 1.00 44.54	N
		NH2 ARG E 503	64.415 45.652 52.881 1.00 43.20	N
		N LEU E 504	62.456 38.159 50.638 1.00 47.24	N
ATOM	9189	CA LEUE 504	61.835 38.066 49.334 1.00 45.05	С

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ATOM	9325	ND2 ASN E 519	41.782 44.115 43.392 1.00 46.73	N
			40,259 48.867 45.721 1.00 45.70	
			39.382 49.814 46.402 1.00 46.05	
ATOM	9328	C LYS E 520	39 572 51 228 45 860 1 00 45 58	
ATOM	9329	O LYS E 520	38.594 51.950 45.722 1.00 45.26	0
			39.722 49.816 47.888 1.00 48.01	С
			40.001 48.371 48.311 1.00 50.52	
ATOM	9332	CD LYS E 520	38.723 47.900 48.965 1.00 54.26	С
ATOM	9333	CE LYS E 520	38.044 46.761 48.220 1.00 56.67	С
			36.608 46.682 48.688 1.00 58.30	
ATOM	9335	N GLY E 521	40.808 51.632 45.554 1.00 44.85	N
ATOM	9336	CA GLY E 521	41.030 52.952 45.003 1.00 45.03	С
			40.250 53.175 43.705 1.00 45.77	
			39.647 54.264 43.636 1.00 45.70	
ATOM	9339	N MET E 522	40.225 52.273 42.702 1.00 45.27	N
ATOM	9340	CA MET E 522	39.478 52.571 41.511 1.00 45.39	С
			37.991 52.603 41.872 1.00 47.59	
			37.272 53.433 41.349 1.00 48.56	
ATOM	9343	CG MET E 522	39.441 51.667 40.334 1.00 45.90	C C
ATOM	9344	CO MET E 522	40.441 50.747 39.785 1.00 47.11 41.710 51.489 38.776 1.00 48.25	S
ATOM	9345	CF MET F 522	40.843 52.867 38.058 1.00 46.66	C
			37.544 51.681 42.724 1.00 49.63	
			36.130 51.710 43.074 1.00 50.27	
			35.820 53.102 43.575 1.00 47.33	
			34.871 53.689 43.113 1.00 48.01	
ATOM	9351	CB GLUE 523	35.797 50.628 44.069 1.00 56.25	С
ATOM	9352	CG GLU E 523	35.392 49.313 43.452 1.00 63.89 34.322 49.449 42.383 1.00 69.24	С
ATOM	9353	CD GLU E 523	34.322 49.449 42.383 1.00 69.24	С
ATOM	9354	OE1 GLU E 523	33.579 50.482 42.394 1.00 72.11	0
			34.219 48.511 41.541 1.00 71.58	Ο
			36.596 53.689 44.450 1.00 44.84	N
			36.385 55.020 44.954 1.00 44.01	C
		C HIS E 524	36.495 56.118 43.922 1.00 44.99	C
		O HIS E 524	35.654 57.015 43.827 1.00 43.85	0
			37.437 55.270 46.046 1.00 43.01	C
		CG HIS E 524	37.353 56.633 46.640 1.00 42.25	C
		ND1 HIS E 524	38.045 57.704 46.130 1.00 43.08	N
		CD2 HIS E 524 CE1 HIS E 524	36.678 57.129 47.680 1.00 42.58 37.801 58.703 46.823 1.00 43.17	C C
		NE2 HIS E 524	37.801 58.793 46.823 1.00 43.17 36.960 58.463 47.792 1.00 42.97	N
		N LEU E 525	37.559 56.112 43.109 1.00 46.94	N N
		CA LEU E 525	37.779 57.153 42.110 1.00 49.17	C
		C LEU E 525	36.580 57.212 41.165 1.00 52.01	c
		O LEU E 525	36.148 58.223 40.631 1.00 52.24	Ö

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ATOM	9415 SG BCYS E 530	28.141 57.575 38.467 0.50 79.92	S
ATOM	9416 N LYS E 531	29.719 61.034 41.209 1.00 81.60	N
ATOM	9417 CA LYS E 531	29.214 62.129 42.002 1.00 83.48	С
ATOM	9418 C LYS E 531	29.595 63.461 41.359 1.00 84.84	С
ATOM	9419 O LYS E 531	29.278 64.547 41.844 1.00 85.98	0
ATOM	9420 CB LYS E 531	29.842 62.116 43.398 1.00 84.16	С
ATOM	9421 CG LYS E 531	29.174 61.255 44.438 1.00 85.42	С
ATOM	9422 CD LYS E 531	28.963 59.818 43.955 1.00 86.01	С
ATOM	9425 N ASN E 532	30.319 63.462 40.270 1.00 86.16	N
ATOM	9426 CA ASN E 532	30.755 64.643 39.563 1.00 87.97	С
ATOM	9427 C ASN E 532	31.574 65.543 40.461 1.00 86.77	С
ATOM	9428 O ASN E 532	31.222 66.693 40.662 1.00 88.13	0
ATOM	9429 CB ASN E 532	29.554 65.398 38.999 1.00 91.01	С
ATOM	9430 CG ASN E 532	28.912 64.605 37.876 1.00 94.27	С
ATOM	9431 OD1 ASN E 532	29.637 64.076 37.022 1.00 95.71	0
ATOM	9432 ND2 ASN E 532	27.576 64.537 37.908 1.00 95.97	N
ATOM	9433 N VALE 533	32.655 65.054 41.021 1.00 85.06	N
ATOM	9434 CA VALE 533	33.541 65.790 41.909 1.00 83.95	С
ATOM	9435 C VAL E 533	34.955 65.844 41.319 1.00 83.81	С
ATOM	9436 O VAL E 533	35.866 66.622 41.603 1.00 84.30	0
ATOM	9437 CB VAL E 533	33.629 65.021 43.246 1.00 83.54	С
ATOM	9438 CG1 VAL E 533	34.400 65.798 44.283 1.00 83.03	С
ATOM	9439 CG2 VAL E 533	32.267 64.604 43.766 1.00 83.52	С
ATOM	9440 N VAL E 534	35.204 64.903 40.422 1.00 82.89	N
ATOM	9441 CA VALE 534	36.458 64.700 39.731 1.00 82.04	, C
ATOM	9442 C VAL E 534	36.409 65.422 38.391 1.00 81.13	С
ATOM	9443 O VAL E 534	35.475 65.259 37.609 1.00 80.09	Ο
ATOM	9444 CB VAL E 534	36.672 63.185 39.430 1.00 82.66	С
		37.826 62.837 38.501 1.00 81.66	С
		36.855 62.411 40.735 1.00 83.03	С
ATOM		37.456 66.179 38.152 1.00 80.63	N
ATOM		37.652 66.898 36.924 1.00 81.29	С
ATOM	9449 C PRO E 535	37.861 65.887 35.797 1.00 82.66	С
	9450 O PRO E 535		Ο
	9451 CB PRO E 535	38.890 67.799 37.083 1.00 80.65	С
		39.350 67.541 38.473 1.00 79.86	С
		38.586 66.375 39.054 1.00 80.52	С
	9454 N LEUE 536	37.723 66.431 34.588 1.00 84.27	N
	9455 CA LEUE 536	37.837 65.722 33.337 1.00 84.25	С
	9456 C LEUE 536	39.244 65.558 32.805 1.00 83.95	C
	9457 O LEUE 536	39.442 65.872 31.616 1.00 85.68	0
	9462 N TYR E 537	40.179 65.068 33.627 1.00 81.54	N
	9463 CA TYR E 537	41.537 64.848 33.115 1.00 78.07	С
	9464 C TYR E 537	41.430 63.607 32.237 1.00 75.64	C
ATOM	9465 O TYR E 537	40.988 62.554 32.656 1.00 74.94	Ο

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АТОМ	9511 CG GLUE 542	42.968 56.080 28.183 1.00 55.43	С
ATOM	9512 CD GLUE 542	44.007 56.740 27.278 1.00 56.20	Č.
ATOM	9513 OE1 GLU E 542	43.863 57.973 27.045 1.00 56.53	Ο
ATOM	9514 OE2 GLU E 542	44.915 56.000 26.861 1.00 56.06	0
ATOM	9515 N MET E 543	42.772 55.618 31.884 1.00 50.13	N
		43.183 54.486 32.707 1.00 50.01	
		42.037 53.999 33.574 1.00 50.73	
ATOM	9518 O MET E 543	41.896 52.801 33.859 1.00 51.88	0
ATOM	9519 CB MET E 543	44.387 54.921 33.546 1.00 50.17	C
		45.472 55.536 32.658 1.00 50.14	
		46.371 54.190 31.854 1.00 49.83	
ATOM	9522 CE MET E 543	46.038 54.596 30.144 1.00 51.73 41.169 54.898 34.041 1.00 50.39	C
ATOM	9523 N LEUE 544	41.109 54.898 34.041 1.00 50.39	N
		40.056 54.453 34.866 1.00 51.08 39.119 53.599 34.022 1.00 52.64	
ATOM	0526 O I FILE 544	38 687 52 545 34 503 1 00 51 80	0
ATOM	9527 CB LEUE 544	39.336 55.621 35.501 1.00 49.82 38.032 55.374 36.237 1.00 49.45	C
ATOM	9528 CG LEU E 544	38.032 55.374 36.237 1.00 49.45	Č
ATOM	9529 CD1 LEU E 544	38.119 54.490 37.461 1.00 48.18	C
ATOM	9530 CD2 LEU E 544	37.470 56.718 36.684 1.00 50.84	С
ATOM	9531 N ASP E 545	38.832 54.032 32.797 1.00 55.61	N
ATOM	9532 CA ASP E 545	38.832 54.032 32.797 1.00 55.61 37.941 53.268 31.941 1.00 59.73	С
ATOM	9533 C ASP E 545	38.457 51.892 31.603 1.00 59.61	С
		37.635 50.985 31.534 1.00 60.30	
ATOM	9535 CB ASP E 545	37.564 53.923 30.628 1.00 64.39	
		36.754 55.196 30.851 1.00 69.96	С
		36.217 55.451 31.975 1.00 71.84	
		36.660 55.974 29.843 1.00 72.34 39.748 51.701 31.435 1.00 60.47	
ATOM	9539 N ALAE 340	40.297 50.385 31.144 1.00 61.70	C
	9541 C ALA E 546		
	9542 O ALA E 546	39.329 48.283 31.712 1.00 63.79	Ō
		41.803 50.399 31.291 1.00 61.61	C
	9544 N HIS E 547	39.719 49.673 33.392 1.00 66.30	N
ATOM	9545 CA HIS E 547	39.225 48.863 34.455 1.00 69.24	C
	9546 C HIS E 547	37.740 48.630 34.433 1.00 73.60	С
	9547 O HIS E 547	37,308 47,495 34,626 1.00 75,89	Ο
	9548 CB HIS E 547	39.532 49.620 35.773 1.00 67.78	C
	9549 CG HIS E 547	40.989 49.285 35.946 1.00 66.33	C
		41.415 48.311 36.802 1.00 66.23	N C
	9551 CD2 HIS E 547 9552 CE1 HIS E 547	42.059 49.802 35.319 1.00 65.84	C
	9553 NE2 HIS E 547	42.729 48.249 36.709 1.00 66.64 43.144 49.133 35.819 1.00 66.16	N
	9554 N ARGE 548	36.961 49.670 34.230 1.00 66.16	N
	9555 CA ARG E 548	35.501 49.450 34.225 1.00 83.82	C
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ATOM 9556 C ARG E 548		С
ATOM 9557 O ARGE 548		Ö
	34.801 50.810 34.241 1.00 87.54	С
ATOM 9559 CG ARG E 548	35.485 51.952 34.980 1.00 90.41	С
ATOM 9560 CD ARG E 548	35.811 51.738 36.443 1.00 93.01	C
ATOM 9561 NE ARG E 548	35.074 50.727 37.193 1.00 95.25	N
	35.442 50.146 38.337 1.00 96.28	C
	36.575 50.450 38.957 1.00 96.79	
	34.660 49.227 38.903 1.00 96.67	N
TER 9565 ARG E 548 HETATM 9566 C1 EST E 600	47.222 60.396 43.519 1.00 34.93	С
HETATM 9566 C1 EST E 600 HETATM 9567 C2 EST E 600	48.571 60.475 43.210 1.00 37.57	C
HETATM 9568 C3 EST E 600	49.436 59.518 43.657 1.00 38.54	Č
HETATM 9569 O3 EST E 600	50.769 59.635 43.327 1.00 40.09	
HETATM 9570 C4 EST E 600	49.033 58.426 44.443 1.00 37.89	Č
HETATM 9571 C5 EST E 600	47.646 58.348 44.751 1.00 36.69	С
HETATM 9572 C6 EST E 600	47.269 57.351 45.831 1.00 35.65	C
HETATM 9573 C7 EST E 600	45.832 57.501 46.268 1.00 34.45	
HETATM 9574 C8 EST E 600	44.938 57.875 45.104 1.00 33.71	C
HETATM 9575 C9 EST E 600	45.317 59.266 44.607 1.00 33.78	С
HETATM 9576 C10 EST E 600		C
HETATM 9577 C11 EST E 600	•	
HETATM 9578 C12 EST E 600	42.980 59.847 43.918 1.00 34.32 42.578 58.437 44.347 1.00 34.56	C
HETATM 9579 C13 EST E 600 HETATM 9580 C14 EST E 600		C
HETATM 9580 C14 EST E 600 HETATM 9581 C15 EST E 600		
HETATM 9582 C16 EST E 600		
HETATM 9583 C17 EST E 600		
HETATM 9584 O17 EST E 600	40.085 58.239 44.257 1.00 35.45	0
HETATM 9585 C18 EST E 600	42.511 57.536 43.119 1.00 34.18	С
ATOM 9586 N SER F 305	54.849 29.184 70.902 1.00 88.75	N
ATOM 9587 CA SER F 305	53.873 28.738 69.869 1.00 88.59	C
ATOM 9588 C SER F 305	54.304 27.466 69.171 1.00 87.91	С
ATOM 9589 O SER F 305	55.423 27.412 68.680 1.00 87.92	0
ATOM 9590 CB SER F 305	53.698 29.871 68.839 1.00 88.47	C O
ATOM 9591 OG SER F 305 ATOM 9592 N LEU F 306	52.794 29.522 67.815 1.00 88.14 53.428 26.475 69.068 1.00 87.84	N
ATOM 9592 N LEU F 306 ATOM 9593 CA LEU F 306	53.764 25.236 68.354 1.00 87.46	C
ATOM 9594 C LEUF 306	54.314 25.700 67.008 1.00 86.18	c
ATOM 9595 O LEU F 306	55.444 25.390 66.663 1.00 86.66	0
ATOM 9596 CB LEUF 306	52.565 24.313 68.117 1.00 88.10	С
ATOM 9600 N ALA F 307	53.519 26.485 66.291 1.00 84.32	N
ATOM 9601 CA ALA F 307	53.906 27.037 65.014 1.00 82.77	С
ATOM 9602 C ALA F 307	55.411 27.233 64.958 1.00 81.44	C
ATOM 9603 O ALA F 307	56.089 26.580 64.173 1.00 81.34	0

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ATOM	9604	CB ALA F 307	53 245 28 399 64 801 1 00 83 53	С
ATOM	9605	N LEUF 308	55.926 28.106 65.806 1.00 80.43	N
			57.349 28.379 65.823 1.00 80.87	С
ATOM	9607	C LEUF 308	58.283 27.248 66.188 1.00 81.37	С
		O LEUF 308		0
			57.544 29.609 66.728 1.00 80.50	С
			56.845 30.879 66.264 1.00 80.59	С
			57.464 32.127 66.851 1.00 80.80	С
		CD2 LEU F 308		С
		N SER F 309		N
		CA SER F 309	58.715 24.939 66.908 1.00 79.92	С
		C SER F 309		C
		O SER F 309		Ο
			58.114 24.299 68.174 1.00 81.24	С
			57.899 25.422 69.018 1.00 85.04	0
			57.616 23.617 65.203 1.00 76.56	N
			57.582 22.522 64.249 1.00 73.92	С
		C LEUF 310		C
			59.173 23.788 62.966 1.00 72.40	0
			56.234 22.376 63.594 1.00 73.55	C
			55.028 22.755 64.432 1.00 72.82	C
		CD1 LEUF 310		C
			54.108 21.571 64.611 1.00 73.65 59.062 21.572 62.657 1.00 71.49	C
			60.116 21.538 61.647 1.00 71.01	N C
			59.429 21.644 60.311 1.00 70.16	c
			58.259 21.238 60.276 1.00 70.11	0
		CB THR F 311		C
			60.069 19.092 61.584 1.00 70.69	O
ATOM	9633	CG2 THR F 311	61.389 20.113 63.250 1.00 71.71	Č
		N ALA F 312		N
		CA ALAF312	59.383 22.153 57.967 1.00 69.06	C
		C ALA F 312	58.565 20.893 57.733 1.00 69.29	c
		O ALA F 312	57.430 20.985 57.256 1.00 69.18	Ö
		CB ALAF312	60.315 22.432 56.817 1.00 69.25	C
		N ASP F 313	59.097 19.728 58.054 1.00 70.53	N
ATOM	9640	CA ASP F 313	58.342 18.498 57.862 1.00 72.19	С
ATOM	9641	C ASP F 313	57.094 18.407 58.701 1.00 70.29	С
ATOM	9642	O ASP F 313	56.062 18.015 58.167 1.00 69.40	0
ATOM	9643	CB ASP F 313	59.258 17.290 58.105 1.00 76.57	С
ATOM	9644	CG ASP F 313	60.094 17.159 56.828 1.00 80.64	C
ATOM	9645	OD1 ASP F 313	59.456 17.019 55.745 1.00 82.23	0
ATOM	9646	OD2 ASP F 313	61.339 17.234 56.980 1.00 82.58	0
ATOM	9647	N GLN F 314	57.138 18.766 59.970 1.00 69.39	N
ATOM	9648	CA GLN F 314	55.944 18.701 60.805 1.00 69.22	С

ATOM 9691 CA LEU F 320 48.275 18.289 55.072 1.00 58.32

51.064 24.328 56.054 1.00 49.82

48.990 24.419 57.502 1.00 49.44

48.861 19.348 55.901 1.00 56.35

47.143 17.594 55.799 1.00 61.15

46.190 17.106 55.215 1.00 61.84

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ATOM 9688 CD1 LEU F 319

ATOM 9689 CD2 LEU F 319

ATOM 9690 N LEUF 320

ATOM 9692 C LEUF 320

ATOM 9693 O LEUF 320

•		325/371	
ATOM	9739 CG1 ILE F 326	35.729 15.472 48.160 1.00 66.76	С
ATOM	9740 CG2 ILE F 326	37.489 17.245 47.925 1.00 64.81	С
ATOM	9741 CD1 ILE F 326	36.186 14.539 49.268 1.00 69.00	С
ATOM	9742 N LEUF 327	33.286 18.514 49.471 1.00 59.83	N
ATOM	9743 CA LEUF 327	31.837 18.354 49.480 1.00 59.01	С
ATOM	9744 C LEUF 327	31.345 17.922 48.116 1.00 60.14	С
	9745 O LEUF 327	32.115 17.939 47.156 1.00 60.86	Ο
ATOM	9746 CB LEUF 327	31.214 19.684 49.901 1.00 57.70	C
ATOM	9747 CG LEUF 327	31.777 20.287 51.182 1.00 57.55	С
ATOM	9748 CD1 LEU F 327	30.782 21.285 51.776 1.00 57.69	С
		32.117 19.257 52.241 1.00 57.43	С
	9750 N TYR F 328	30.089 17.529 47.994 1.00 61.33	N
ATOM	9751 CA TYR F 328	29.522 17.172 46.703 1.00 62.52	С
ATOM	9752 C TYR F 328	28.386 18.181 46.541 1.00 63.58	С
ATOM	9753 O TYR F 328	27.787 18.516 47.561 1.00 63.48	Ο
ATOM	9754 CB TYR F 328	28.866 15.796 46.605 1.00 63.71	С
ATOM	9755 CG TYR F 328	29.933 14.732 46.471 1.00 64.32	С
		30.548 14.151 47.562 1.00 64.90	C
ATOM	9757 CD2 TYR F 328	30.317 14.351 45.203 1.00 64.90	C
ATOM	9758 CE1 TYR F 328	31.533 13.198 47.392 1.00 66.06	C
ATOM	9759 CE2 TYR F 328	31.295 13.395 45.025 1.00 65.70	С
ATOM	9760 CZ TYR F 328		C
	9761 OH TYR F 328	32,889 11.890 45.884 1.00 68.16	0
	9762 N SER F 329	28.133 18.592 45.333 1.00 65.88	N
ATOM	9763 CA SER F 329	27.054 19.541 45.092 1.00 68.50	С
	9764 C SER F 329	25.712 18.825 45.264 1.00 71.15	C
ATOM	9765 O SER F 329	25.556 17.659 44.962 1.00 69.43	0
ATOM	9766 CB SER F 329	27.102 20.126 43.683 1.00 68.03	C
		25.839 20.726 43.440 1.00 68.18	0
ATOM	9768 N GLUF 330	24.743 19.570 45.772 1.00 76.47	N
		23.389 19.115 46.031 1.00 80.61	C
	9770 C GLU F 330	22.727 18.695 44.721 1.00 81.23	C
	9771 O GLUF 330	22.859 19.388 43.715 1.00 82.27	0
	9772 CB GLUF 330	22.589 20.215 46.728 1.00 84.17	C
	9773 CG GLU F 330	21.383 20.767 45.992 1.00 88.92	C
	9774 CD GLU F 330	21.510 22.185 45.467 1.00 91.99	C
	9775 OE1 GLU F 330	21.304 23.149 46.266 1.00 93.25	C
	9776 OE2 GLU F 330	21.809 22.337 44.246 1.00 93.41	C
	9777 N PHE F 337	19.883 24.928 34.219 1.00 86.00	N
	9778 CA PHE F 337	20.742 25.994 34.681 1.00 85.03	C
	9779 C PHE F 337	20.201 27.364 34.287 1.00 83.38	C
ATOM		20.007 27.566 33.099 1.00 83.77	0
ATOM		22.159 25.935 34.088 1.00 85.89	C
	9782 CG PHE F 337	23.038 25.026 34.898 1.00 87.17	C
ATOM	9783 CD1 PHE F 337	22.817 24.805 36.239 1.00 87.56	C

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ATOM	9784 CD2 PHE F'337	24.095 24.380 34.276 1.00 87.89	С
ATOM	9785 CE1 PHE F 337	23.642 23.957 36.942 1.00 88.83	Ċ
ATOM	9786 CE2 PHE F 337	24.929 23.526 34.962 1.00 88.18	С
		24.698 23.318 36.308 1.00 89.08	
ATOM	9788 N SER F 338	20.037 28.218 35.270 1.00 80.62	N
		19.577 29.573 34.995 1.00 78.22	
		20.401 30.467 35.897 1.00 76.60 20.845 29.967 36.939 1.00 76.99	
ATOM	9792 CB SER F 338	18.088 29.667 35.311 1.00 78.08	C
ATOM	9793 OG SER F 338	18.088 29.667 35.311 1.00 78.08 17.785 29.015 36.523 1.00 77.58	Ö
ATOM	9794 N GLUF 339	20.575 31.736 35.600 1.00 74.82	N
ATOM	9795 CA GLUF 339	21.318 32.604 36.534 1.00 73.09	С
ATOM	9796 C GLUF 339	20.939 32.174 37.951 1.00 71.30 21.769 31.721 38.735 1.00 70.30	C
ATOM	9797 O GLUF 339	21.769 31.721 38.735 1.00 70.30	O C
		20.958 34.040 36.203 1.00 73.57 21.102 35.120 37.254 1.00 74.18	
ATOM	9800 CD GLU F 339	21.495 36.392 36.517 1 00 75 77	C
ATOM	9801 OE1 GLUF 339	22.483 36.313 35.744 1.00 75.89	Ō
ATOM	9802 OE2 GLU F 339	20.817 37.433 36.705 1.00 77.28	0
		19.648 32.249 38.293 1.00 69.59	
ATOM	9804 CA ALAF 340	19.192 31.861 39.607 1.00 67.96	C
		19.566 30.438 39.970 1.00 66.96	
		20.091 30.235 41.066 1.00 68.75 17.687 32.024 39.737 1.00 67.62	
		19.302 29.459 39.142 1.00 65.15	
ATOM	9809 CA SER F 341	19.618 28.088 39.529 1.00 65.19	C
ATOM	9810 C SER F 341	21.108 27.902 39.705 1.00 63.98	С
		21.522 27.252 40.673 1.00 64.74	
ATOM	9812 CB SER F 341	19.004 27.077 38.566 1.00 67.22	C
	9813 OG SER F 341 9814 N MET F 342	19.940 26.356 37.790 1.00 69.32	
		21.937 28.429 38.812 1.00 62.49 23.380 28.262 38.976 1.00 60.83	N C
	9816 C MET F 342		c
	9817 O MET F 342		Ö
ATOM	9818 CB MET F 342	24.168 28.719 37.751 1.00 60.66	С
	9819 CG MET F 342	25.596 28.200 37.887 1.00 61.87	С
	9820 SD MET F 342	26.497 28.176 36.308 1.00 63.51	S
	9821 CE MET F 342 9822 N MET F 343	26.629 29.935 36.028 1.00 62.32 23.563 30.272 40.396 1.00 58.10	C
	9823 CA MET F 343	24.029 31.011 41.555 1.00 56.16	N C
	9824 C MET F 343	23,676 30.186 42.780 1.00 56.22	c
	9825 O MET F 343	24.486 30.013 43.683 1.00 57.06	Ö
ATOM	9826 CB MET F 343	23.404 32.383 41.634 1.00 56.11	С
		24.093 33.365 40.708 1.00 56.34	С
ATOM	9828 SD MET F 343	25.845 33.433 41.051 1.00 56.93	S

			2011	
			25.848 33.732 42.820 1.00 55.38	
			22.460 29.655 42.797 1.00 55.26	
			22.027 28.824 43.901 1.00 54.47	
		C GLYF 344		С
		O GLY F 344		О
			23.372 26.851 43.267 1.00 53.87	N
ATOM	9835	CA LEUF 345	24.314 25.771 43.552 1.00 53.39	С
			25.656 26.242 44.104 1.00 52.00	С
		O LEUF 345		О
			24.739 25.014 42.299 1.00 54.69	С
			23.653 24.140 41.677 1.00 57.12	С
ATOM	9840	CD1 LEU F 345	23.450 24.634 40.246 1.00 57.95	С
			24.072 22.682 41.765 1.00 57.27	С
			26.249 27.134 43.309 1.00 49.99	N
			27.546 27.717 43.623 1.00 47.43	C
ATOM	9844	C LEUF 346	27.526 28.269 45.029 1.00 46.98	С
			28.261 27.925 45.955 1.00 46.10	Ο
			27.764 28.728 42.499 1.00 46.52	С
			28.182 28.091 41.178 1.00 46.34	С
			28.806 29.155 40.289 1.00 47.33	С
			29.175 26.943 41.340 1.00 46.14	С
			26.562 29.149 45.243 1.00 46.52	N
ATOM	9851	CA THR F 347	26.333 29.794 46.530 1.00 46.62	C
			26.099 28.809 47.631 1.00 47.13	C
			26.665 28.944 48.703 1.00 48.40	О
			25.182 30.771 46.232 1.00 46.91	С
			25.774 32.084 46.378 1.00 49.31	О
			23.919 30.552 46.981 1.00 44.84	С
			25.305 27.770 47.451 1.00 48.46	N
			25.022 26.738 48.432 1.00 48.26	С
			26.307 26.002 48.775 1.00 46.59	C
		O ASN F 348	26.704 25.822 49.913 1.00 47.10	0
			24.011 25.751 47.845 1.00 51.69	C
		CG ASN F 348	23.760 24.555 48.771 1.00 55.48	C
		OD1 ASN F 348	24.408 23.479 48.722 1.00 55.42	0
		ND2 ASN F 348	22.764 24.796 49.662 1.00 56.81	N
		N LEUF 349	27.026 25.552 47.772 1.00 45.09	N
		CA LEUF 349	28.291 24.853 47.949 1.00 43.71	С
		C LEU F 349	29.231 25.731 48.767 1.00 42.81	C
		O LEUF 349	29.848 25.257 49.723 1.00 42.31	0
		CB LEUF 349	28.830 24.503 46.549 1.00 44.45	C
		CG LEUF 349	30.133 23.716 46.557 1.00 45.86	C
		CD1 LEU F 349	29.887 22.339 47.210 1.00 46.82	C
		•	30.750 23.524 45.196 1.00 46.02	С
ATOM	9873	N ALAF350	29.345 27.026 48.466 1.00 41.52	N

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ATOM	9919	CG1 VAL F 355	30.568 23.938 59.191 1.00 40.99	С
ATOM	9920	CG2 VAL F 355	29.276 25.541 57.764 1.00 42.17	С
ATOM	9921	N HIS F 356	33,363 24,019 56,985 1.00 43.95	N
ATOM	9922	CA HISF 356	34.607 23.267 57.066 1.00 45.14	С
			35.765 24.222 57.213 1.00 44.30	С
ATOM	9924	O HIS F 356	36.682 24.016 58.008 1.00 44.09	Ο
ATOM	9925	CB HIS F 356	34.690 22.340 55.844 1.00 48.01	С
ATOM	9926	CG HIS F 356	33.569 21.342 55.974 1.00 51.72	С
ATOM	9927	ND1 HIS F 356	33.751 20.044 56.403 1.00 53.60	N
ATOM	9928	CD2 HIS F 356	32.240 21.467 55.770 1.00 53.10	С
ATOM	9929	CE1 HIS F 356	32,580 19,434 56,435 1,00 53,89	С
ATOM	9930	NE2 HIS F 356	31.634 20.265 56.056 1.00 53.29	N
ATOM	9931	N MET F 357	35.728 25.311 56.441 1.00 43.92	N
ATOM			36.797 26.279 56.449 1.00 43.10	С
ATOM	9933	C MET F 357	37.175 26.739 57.856 1.00 43.05	С
ATOM			38.354 26.763 58.204 1.00 43.76	О
ATOM	9935	CB MET F 357	36.486 27.554 55.656 1.00 42.86	С
ATOM	9936	CG MET F 357	37.813 28.308 55.484 1.00 42.98	С
ATOM	9937	SD MET F 357	37.574 29.868 54.643 1.00 43.25	S
ATOM	9938	CE MET F 357	37.137 29.259 52.991 1.00 43.78	С
ATOM	9939	N ILEF 358	36.174 27.137 58.616 1.00 41.67	N
ATOM	9940	CA ILE F 358	36.371 27.608 59.972 1.00 41.23	С
ATOM	9941	C ILE F 358	37.132 26.581 60.781 1.00 42.66	С
ATOM	9942	O ILE F 358	38.079 26.929 61.491 1.00 43.00	0
ATOM	9943	CB ILE F 358	35.003 27.877 60.634 1.00 39.57	С
ATOM	9944	CG1 ILE F 358	34.325 28.975 59.814 1.00 39.81	С
ATOM			35.123 28.255 62.078 1.00 37.70	С
ATOM	9946	CD1 ILE F 358	32.999 29.421 60.382 1.00 41.24	С
ATOM	9947	N ASN F 359		N
ATOM	9948	CA ASN F 359	37.375 24.250 61.394 1.00 47.81	С
ATOM		C ASN F 359		С
ATOM		O ASN F 359		О
			36.696 22.907 61.058 1.00 52.88	С
		CG ASN F 359		С
			35.709 22.917 63.097 1.00 60.88	. 0
		ND2 ASN F 359		N
		N TRP F 360	39.023 24.078 59.653 1.00 43.52	N
		CA TRP F 360	40.373 24.013 59.131 1.00 42.62	С
		C TRP F 360	41.264 25.111 59.670 1.00 42.88	C
		O TRP F 360	42.406 24.935 60.061 1.00 42.92	O
		CB TRP F 360	40.226 24.186 57.614 1.00 42.66	C
		CG TRP F 360	41.553 24.512 57.001 1.00 42.12	C
		CD1 TRP F 360	42.551 23.635 56.778 1.00 41.75	C
		CD2 TRP F 360	41.999 25.803 56.561 1.00 42.44	C
ATOM	9963	NEI TRP F 360	43.590 24.317 56.218 1.00 43.62	N

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АТОМ	9964 CE2 TRP F 360	43.299 25.645 56.061 1.00 42.40	С
		41.419 27.082 56.547 1.00 42.27	
		44.067 26.675 55.548 1.00 41.65	
ATOM	9967 CZ3 TRP F 360	42.177 28.116 56.036 1.00 42.74	С
ATOM	9968 CH2 TRP F 360	43.478 27.906 55.548 1.00 42.73	С
		40.770 26.351 59.666 1.00 44.32	N
		41.496 27.515 60.143 1.00 44.21	С
		42.042 27.224 61.523 1.00 45.40	С
		43.218 27.491 61.736 1.00 45.18	0
		40.612 28.740 60.157 1.00 43.35	
	9974 N LYS F 362		N
		41.695 26.383 63.771 1.00 50.51	C
		42.934 25.524 63.877 1.00 50.52 43.657 25.648 64.864 1.00 50.40	C O
ATOM	9977 O LIST 302	40.524 25.801 64.571 1.00 53.28	C
		39.434 26.852 64.802 1.00 56.10	Č
		39.915 27.861 65.822 1.00 58.93	
		38.881 28.178 66.898 1.00 61.09	
		39.409 29.008 68.036 1.00 61.11	
		43,241 24.677 62.936 1.00 50.76	
		44.398 23.836 62.900 1.00 52.41	
ATOM	9985 C ARG F 363	45.589 24.400 62.149 1.00 51.42	С
ATOM	9986 O ARG F 363	46.595 23.700 62.027 1.00 52.42	0
		44.027 22.559 62.132 1.00 57.14	
		42.522 22.408 62.005 1.00 63.12	
ATOM	9989 CD ARG F 363	42.037 21.691 63.293 1.00 69.42	C
		42.619 20.335 63.225 1.00 75.02	
		42.205 19.469 62.282 1.00 78.35	
		41.238 19.854 61.445 1.00 79.78 42.748 18.249 62.182 1.00 79.54	
	9994 N VAL F 364		N
	9995 CA VAL F 364	46.754 26.080 60.871 1.00 47.95	C
	9996 C VAL F 364	47.689 26,535 61.964 1.00 47.06	C
	9997 O VAL F 364	47.364 27.425 62.733 1.00 47.62	0
ATOM	9998 CB VALF 364	46.336 27.238 59.945 1.00 46.96	С
ATOM	9999 CG1 VAL F 364	47.520 27.990 59.395 1.00 46.14	С
ATOM	10000 CG2 VAL F 364		С
	10001 N PRO F 365	48.834 25.947 62.111 1.00 46.86	N
	10002 CA PRO F 365	49.795 26.303 63.142 1.00 47.30	С
	10003 C PROF 365	49.914 27.803 63.280 1.00 47.97	C
	10004 O PRO F 365	50.102 28.494 62.282 1.00 49.63	0
	10005 CB PRO F 365	51.119 25.617 62.755 1.00 46.66	C
	10006 CG PRO F 365 10007 CD PRO F 365	50.541 24.380 62.100 1.00 47.21	C C
	10007 CD PRO F 365 10008 N GLY F 366	49.314 24.832 61.289 1.00 47.57 49.771 28.338 64.487 1.00 48.33	N
ATUM	10006 IN GLIF 300	47.//1 20.330 04.48/ 1.00 40.33	14

			3511311	
			49.879 29.737 64.813 1.00 47.57	С
		C GLY F 366	48.589 30.521 64.858 1.00 47.62	С
		O GLY F 366	48.493 31.600 65.468 1.00 48.03	О
ATOM	10012	N PHE F 367	47,562 30.022 64.184 1.00 46.85	N
ATOM	10013	CA PHE F 367	46.281 30.718 64.081 1.00 46.59	С
ATOM	10014	C PHE F 367	45.595 30.997 65.410 1.00 46.36	С
ATOM	10015	O PHE F 367	45.152 32.047 65.848 1.00 45.52	Ο
ATOM	10016	CB PHE F 367	45.325 29.920 63.189 1.00 44.75	С
ATOM	10017	CG PHE F 367	44.071 30.654 62.850 1.00 44.60	С
ATOM	10018	CD1 PHE F 367	44.073 31.662 61.912 1.00 44.16	С
ATOM	10019	CD2 PHE F 367	42.875 30.334 63.491 1.00 45.67	С
			42.919 32.340 61.592 1.00 44.81	С
			41.696 30.997 63.180 1.00 45.38	С
ATOM	10022	CZ PHE F 367	41.723 31.996 62.222 1.00 45.46	C
		N VALF368	45.510 29.919 66.150 1.00 46.98	N
			44.884 29.809 67.454 1.00 47.50	С
		C VAL F 368	45.555 30.694 68.470 1.00 48.39	С
		O VAL F 368	44.887 31.054 69.446 1.00 49.08	Ο
		CB VALF 368	44.845 28.309 67.816 1.00 46.46	C
		_ _	45.352 28.034 69.195 1.00 46.31	C
		CG2 VAL F 368	43.434 27.799 67.573 1.00 46.30	C
		N ASP F 369	46.810 31.080 68.264 1.00 48.91	N
		CA ASP F 369	47.504 31.989 69.146 1.00 49.05	C
		C ASP F 369	46.994 33.411 68.959 1.00 48.03	C
		O ASP F 369	47.416 34.260 69.730 1.00 49.36	0
		CB ASP F 369	49.005 32.039 68.908 1.00 52.31	C
		CG ASP F 369	49.679 30.684 68.963 1.00 56.87	C
		OD1 ASP F 369	49.349 29.868 69.872 1.00 59.10	0
		OD2 ASP F 369	50.566 30.390 68.109 1.00 57.95	0
		N LEUF 370	46.158 33.800 68.021 1.00 46.74	N C
		CA LEUF 370	45.655 35.163 67.888 1.00 44.48	c
		C LEUF 370	44.419 35.379 68.749 1.00 42.98 43.795 34.398 69.161 1.00 42.49	0
		O LEUF 370		
			45.321 35.373 66.403 1.00 45.02 46.514 35.297 65.452 1.00 45.13	C
		CG LEUF 370	46.314 33.297 63.432 1.00 43.13	C
		CD1 LEU F 370	47.506 36.398 65.830 1.00 45.41	C
		CD2 LEU F 370 N THR F 371	44.016 36.601 69.059 1.00 41.35	N
		CA THR F 371	42.833 36.757 69.881 1.00 40.62	C
		C THR F 371	42.833 36.737 69.881 1.00 40.02	c
		O THR F 371	41.627 36.260 67.864 1.00 42.62	Ö
		CB THR F 371	42.575 38.216 70.192 1.00 40.25	C
		OG1 THR F 371	42.575 38.216 70.192 1.00 40.25	0
		CG2 THR F 371	43.594 38.781 71.114 1.00 40.04	C
		N LEUF 372	40.602 35.837 69.761 1.00 44.21	N
ATOM	10023	N LEUF 3/2	40.002 33.037 03.701 1.00 44.21	14

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ATOM	10054	CA LEUF 372	39.418 35.325 69.102 1.00 44.26	С
ATOM	10055	C LEUF 372	39.418 35.325 69.102 1.00 44.26 38.932 36.292 68.047 1.00 45.09	С
ATOM	10056	O LEU F 372	38.550 35.821 66.966 1.00 46.27	0
ATOM	10057	CB LEUF 372	38.388 35.012 70.186 1.00 43.22	С
ATOM	10058	CG LEUF 372	38.740 33.838 71.093 1.00 41.50	С
ATOM	10059	CD1 LEU F 372	37.680 33.752 72.173 1.00 42.51	C
			38.762 32.559 70.291 1.00 40.77	С
			38.935 37.602 68.274 1.00 45.60	N
ATOM	10062	CA HIS F 373	38.399 38.491 67.238 1.00 46.42	С
ATOM	10063	C HIS F 373	39.328 38.508 66.059 1.00 45.56	С
			38.840 38.440 64.937 1.00 44.91	
			38.048 39.845 67.807 1.00 49.57	
ATOM	10066	CG HIS F 373	36.763 39.812 68.579 1.00 52.32	С
			36.676 39.816 69.958 1.00 53.50	
			35.497 39.767 68.163 1.00 53.33	
ATOM	10069	CE1 HIS F 373	35.408 39.782 70.315 1.00 54.25	C
ATOM	10070	NE2 HIS F 373	34.653 39.741 69.241 1.00 54.69 40.637 38.530 66.279 1.00 45.43	N
ATOM	10071	N ASP F 374	40.637 38.530 66.279 1.00 45.43	N
			41.558 38.487 65.134 1.00 44.42	
			41.355 37.269 64.272 1.00 43.20	
			41.438 37.415 63.053 1.00 43.11	0
			43.004 38.647 65.603 1.00 45.47	C
			43.075 40.126 65.975 1.00 48.30	
			42.115 40.854 65.579 1.00 48.90	
			44.051 40.564 66.632 1.00 50.38	
		N GLNF 375		
			40.791 34.951 64.031 1.00 42.84	
			39.583 35.269 63.159 1.00 43.36 39.619 35.161 61.925 1.00 43.87	
ATOM	10082	CD CINE 275	40.583 33.750 64.914 1.00 43.60	0
ATOM	10083	CG GINE 275	40.383 33.730 04.914 1.00 43.00	C C
		CD GLN F 375	41.827 33.439 65.729 1.00 45.60 41.568 32.352 66.757 1.00 46.87	C
		OE1 GLN F 375	40.780 31.422 66.560 1.00 47.29	0
		NE2 GLN F 375	42.244 32.497 67.888 1.00 47.07	N
		N VAL F 376	38.496 35.752 63.774 1.00 43.02	N
		CA VALF 376	37.322 36.091 62.969 1.00 42.27	C
		C VAL F 376	37.749 37.033 61.861 1.00 42.22	c
		O VAL F 376	37.412 36.808 60.705 1.00 43.67	Ö
		CB VALF 376	36.139 36.621 63.764 1.00 41.25	C
		CG1 VAL F 376	34.885 36.524 62.909 1.00 42.60	C
		CG2 VAL F 376	35.858 35.782 64.983 1.00 40.27	Č
		N HIS F 377	38.514 38.062 62.146 1.00 42.99	N
		CA HISF 377	39.001 38.986 61.129 1.00 43.28	C
		C HIS F 377	39.765 38.268 60.046 1.00 42.83	C
· -		O HIS F 377	39.285 38.351 58.901 1.00 43.87	O

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			333/371	_
		CB HIS F 377		С
			40.368 41.134 60.835 0.50 43.00	C
		CG BHIS F 377		C N
			38.930 41.315 63.832 0.50 45.60	
ATOM	10103	CD2AHIS F 377	41 632 41 377 60 432 0 50 43 02	C
ATOM	10105	CD2BHIS F 377	41.632 41.377 60.432 0.50 43.02 37.684 41.620 62.069 0.50 45.70	Č
ATOM	10106	CE1AHIS F 377	40.346 42.832 59.421 0.50 42.88	č
			37.937 42.103 64.205 0.50 45.09	
			41.595 42.430 59.546 0.50 42.80	
ATOM	10109	NE2BHIS F 377	37.168 42.296 63.156 0.50 45.46	N
ATOM	10110	N LEUF 378	40.848 37.528 60.241 1.00 41.51	N
			41.470 36.883 59.064 1.00 40.44	
		C LEUF 378		C .
			40.382 36.020 57.037 1.00 38.68	0
			42.724 36.129 59.482 1.00 41.23	C C
			43.717 36.893 60.386 1.00 40.82 44.893 36.008 60.747 1.00 40.06	C
			44.199 38.162 59.734 1.00 39.28	C
			39.601 35.307 58.975 1.00 40.27	N
			38.587 34.518 58.288 1.00 39.44	C
ATOM	10120	C LEUF 379	37.741 35.406 57.400 1.00 39.11	C
ATOM	10121	O LEUF 379	37.741 35.406 57.400 1.00 39.11 37.741 35.194 56.193 1.00 38.45	0
ATOM	10122	CB LEU F 379	37.725 33.772 59.296 1.00 39.11	C
			38.318 32.362 59.508 1.00 40.15	С
ATOM	10124	CD1 LEU F 379	37.441 31.705 60.581 1.00 40.96	C
			38.438 31.556 58.227 1.00 38.06	C
			37.082 36.405 57.990 1.00 39.47 36.254 37.307 57.205 1.00 40.79	N C
			37.051 37.901 56.056 1.00 42.77	c
		O GLU F 380		Ö
ATOM	10130	CB GLUF 380	35.715 38.422 58.054 1.00 40.39	C
		CG GLUF 380	34.729 37.959 59.122 1.00 43.41	С
ATOM	10132	CD GLUF 380	34.453 39.151 60.011 1.00 44.98	С
ATOM	10133	OE1 GLU F 380	35.364 40.007 60.152 1.00 47.79	0
		OE2 GLU F 380	33.374 39.296 60.582 1.00 46.00	0
		N CYS F 381	38.303 38.264 56.267 1.00 44.51	N
			39.090 38.839 55.214 1.00 45.77	C
		C CYS F 381	39.431 37.884 54.107 1.00 43.13	C
		O CYS F 381 CB CYS F 381	39.293 38.321 52.966 1.00 41.88 40.286 39.552 55.869 1.00 50.51	O C
		SG CYS F 381	40.155 41.305 55.384 1.00 63.88	S
		N ALA F 382	39.868 36.656 54.352 1.00 40.87	N
		CA ALAF 382	40.259 35.766 53.266 1.00 39.08	C
		C ALA F 382	39.347 34.668 52.779 1.00 39.12	C

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ATOM	10144	O ALA F 382	39.688 33.906 51.885 1.00 38.15	0
ATOM	10145	CB ALAF382	39.688 33.906 51.885 1.00 38.15 41.475 35.039 53.859 1.00 37.88	С
ATOM	10146	N TRP F 383	38.133 34.521 53.295 1.00 40.06	N
			37.225 33.440 52.930 1.00 38.49	
ATOM	10148	C TRP F 383	37.151 33.142 51.460 1.00 38.16	С
			37.467 32.026 51.053 1.00 38.73	0
ATOM	10150	CB TRP F 383	35.880 33.677 53.561 1.00 38.28	С
ATOM	10151	CG TRP F 383	35.000 34.712 52.953 1.00 37.76 34.895 36.036 53.260 1.00 36.51	С
ATOM	10152	CD1 TRP F 383	34.895 36.036 53.260 1.00 36.51	С
ATOM	10153	CD2 TRP F 383	34.053 34.447 51.908 1.00 37.63	С
ATOM	10154	NE1 TRP F 383	33.945 36.613 52.468 1.00 36.21	N
ATOM	10155	CE2 TRP F 383	33.420 35.675 51.625 1.00 37.28	С
ATOM	10156	CE3 TRP F 383	33.719 33.295 51.188 1.00 37.36	С
ATOM	10157	CZ2 TRP F 383	32.449 35.775 50.636 1.00 37.38	C
ATOM	10158	CZ3 TRP F 383	32.753 33.408 50.211 1.00 37.26	C
ATOM	10159	CH2 TRP F 383	32.131 34.632 49.957 1.00 37.38 36.788 34.113 50.637 1.00 38.14	С
ATOM	10160	N LEUF 384	36.788 34.113 50.637 1.00 38.14	N
			36.696 33.901 49.194 1.00 36.05	
			38.052 33.633 48.585 1.00 35.25	
ATOM	10163	O LEUF 384	38.125 32.851 47.649 1.00 34.43	0
ATOM	10164	CB LEUF 384	35.928 35.038 48.559 1.00 35.43	C C
			35.605 34.908 47.078 1.00 35.80 34.913 33.586 46.766 1.00 36.21	C
			34.696 36.047 46.633 1.00 35.95	
		N GLUF 385		
			40.474 33.902 48.470 1.00 36.48	
		C GLU F 385		
			41.082 31.709 47.798 1.00 36.28	
ATOM	10172	CB GLU F 385	41.621 34.721 49.025 1.00 36.55	C
ATOM	10173	CG GLUF 385	41.919 36.044 48.377 1.00 37.81	С
			42.997 36.840 49.082 1.00 40.00	С
		OE1 GLU F 385		O
		OE2 GLU F 385		Ο
ATOM	10177	N ILE F 386	40.491 31.950 49.952 1.00 36.53	. N
ATOM	10178	CA ILE F 386	40.640 30.554 50.291 1.00 37.02	С
ATOM	10179	C ILE F 386	39.749 29.686 49.389 1.00 37.09	С
ATOM	10180	O ILE F 386	40.229 28.726 48.783 1.00 36.20	Ο
		CB ILEF386	40.250 30.145 51.708 1.00 37.27	С
		CG1 ILE F 386	40.796 31.053 52.794 1.00 39.60	С
		CG2 ILE F 386	40.758 28.731 51.927 1.00 37.45	C
		CD1 ILE F 386	42.314 31.140 52.836 1.00 40.65	C
		N LEUF 387	38.458 29.998 49.293 1.00 37.75	N
		CA LEUF 387	37.599 29.211 48.423 1.00 38.77	С
		C LEUF 387	38.125 29.170 46.978 1.00 39.37	C
ATOM	10188	O LEUF 387	38.066 28.107 46.352 1.00 40.51	Ο

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ATOM 10189 CB I FILE 387	36.179 29.739 48.301 1.00 38.25	С
ATOM 10190 CG LEUF 387	35.216 29.455 49.431 1.00 40.30	Č
ATOM 10191 CD1 LEUF 387	33.877 30.170 49.167 1.00 39.62	С
	35.021 27.953 49.664 1.00 40.61	
ATOM 10193 N MET F 388	38.604 30.290 46.438 1.00 38.48	N
ATOM 10194 CA MET F 388	39.063 30.328 45.065 1.00 37.19	С
	40.347 29.550 44.876 1.00 37.70	
	40.429 28.826 43.872 1.00 37.76	
ATOM 10197 CB MET F 388	39.209 31.722 44.481 1.00 36.71	C
ATOM 10198 CG MET F 388	38.093 32.711 44.661 1.00 37.34	C
	38.116 34.146 43.573 1.00 37.46	
	36.408 34.579 43.449 1.00 37.42	
	41.331 29.621 45.769 1.00 38.65	
ATOM 10202 CA ILEF 389	42.550 28.825 45.480 1.00 39.81	
	42.209 27.328 45.536 1.00 41.13 42.756 26.498 44.820 1.00 41.83	
ATOM 10204 O ILE F 389	43.733 29.218 46.362 1.00 38.00	C
ATOM 10203 CB ILEF 389	45.011 28.484 45.961 1.00 36.25	C
ATOM 10200 CG1 ILE1 389	43.441 28.950 47.825 1.00 37.53	Č
ATOM 10208 CD1 ILE F 389	46.257 29.160 46.487 1.00 34.71	
ATOM 10209 N GLY F 390	41.258 26.930 46.367 1.00 41.24	N
ATOM 10210 CA GLY F 390	40.864 25.547 46.457 1.00 42.91	С
ATOM 10211 C GLY F 390	40.313 25.110 45.108 1.00 43.54	C
	40.759 24.117 44.531 1.00 44.30	
ATOM 10213 N LEUF 391	39.335 25.876 44.627 1.00 43.05	N
ATOM 10214 CA LEUF 391	38.711 25.540 43.353 1.00 42.22	C
ATOM 10215 C LEUF 391	39.783 25.406 42.300 1.00 43.71	C
	39.885 24.426 41.583 1.00 44.85	
ATOM 10217 CB LEUF 391	37.798 26.671 42.935 1.00 42.46	C C
ATOM 10218 CG LEUF 391	37.214 26.653 41.542 1.00 43.85 36.455 25.339 41.330 1.00 45.13	C
ATOM 10219 CD1 LEU F 391 ATOM 10220 CD2 LEU F 391		C
ATOM 10220 CD2 LEG F 391 ATOM 10221 N VAL F 392		N
ATOM 10221 IN VALIF 392		C
ATOM 10223 C VAL F 392	42.489 25.157 41.261 1.00 45.06	C
ATOM 10224 O VAL F 392		0
ATOM 10225 CB VAL F 392	42.579 27.696 41.315 1.00 42.58	С
ATOM 10226 CG1 VAL F 392	43.823 27.562 40.465 1.00 42.02	C
ATOM 10227 CG2 VAL F 392		C
ATOM 10228 N TRP F 393	42.937 24.863 42.454 1.00 46.09	N
ATOM 10229 CA TRP F 393	43.769 23.684 42.706 1.00 48.55	C
ATOM 10230 C TRP F 393	43.100 22.384 42.329 1.00 49.16	C
ATOM 10231 O TRP F 393	43.742 21.554 41.700 1.00 51.40	0
ATOM 10232 CB TRP F 393		C C
ATOM 10233 CG TRP F 393	44.508 22.284 44.664 1.00 49.21	C

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ATOM 10234 CD1 TRP F 393	43.801 21.410 45.415 1.00 49.59	С
ATOM 10235 CD2 TRP F 393	45.758 21.664 44.369 1.00 49.88	С
ATOM 10236 NE1 TRP F 393	45.758 21.664 44.369 1.00 49.88 44.549 20.265 45.633 1.00 50.00	N
ATOM 10237 CE2 TRP F 393	45.752 20.398 45.004 1.00 49.70	С
ATOM 10238 CE3 TRP F 393	46.888 22.060 43.645 1.00 50.21	С
ATOM 10239 CZ2 TRP F 393	46 827 19.523 44.939 1.00 49.76	С
ATOM 10240 CZ3 TRP F 393	47.960 21.179 43.580 1.00 50.79	С
ATOM 10241 CH2 TRP F 393	47.920 19.925 44.223 1.00 50.52	С
ATOM 10242 N ARG F 394	41.848 22.202 42.736 1.00 48.49	N
ATOM 10243 CA ARG F 394	41.168 20.977 42.363 1.00 48.26 40.768 21.048 40.897 1.00 49.54	С
ATOM 10244 C ARG F 394	40.768 21.048 40.897 1.00 49.54	С
ATOM 10245 O ARG F 394	40.361 20.055 40.307 1.00 51.77	0
ATOM 10246 CB ARG F 394	39.961 20.631 43.203 1.00 47.19	С
ATOM 10247 CG ARG F 394	38.965 21.623 43.674 1.00 45.48	С
ATOM 10248 CD ARG F 394	37.928 20.983 44.585 1.00 44.46	С
ATOM 10249 NE ARG F 394	36.762 21.872 44.620 1.00 46.03	N
ATOM 10250 CZ ARG F 394	36.680 22.973 45.370 1.00 44.99 4 37.755 23.200 46.108 1.00 44.94	С
ATOM 10251 NH1 ARG F 39	4 37.755 23.200 46.108 1.00 44.94	N
	4 35.631 23.780 45.357 1.00 43.48	
	40.842 22.169 40.217 1.00 50.68	
	40.450 22.232 38.826 1.00 52.13	
ATOM 10255 C SER F 395	41.637 22.045 37.903 1.00 54.26	C
	41.430 22.047 36.690 1.00 54.51	
	39.814 23.613 38.598 1.00 51.54 38.434 23.568 38.917 1.00 49.50	
ATOM 10250 N. MET F 206	42.841 21.927 38.429 1.00 56.83	N
ATOM 10259 N MET F 396	44.049 21.787 37.662 1.00 60.12	, C
ATOM 10261 C MET F 396	44.093 20.804 36.507 1.00 63.54	Č
	44.429 21.178 35.366 1.00 64.11	
ATOM 10262 CB MET F 396	45 163 21 300 38 583 1 00 60 15	C
ATOM 10264 CG MET F 396	45.163 21.300 38.583 1.00 60.15 46.413 22.143 38.424 1.00 60.96	Č
ATOM 10265 SD MET F 396	47.220 22.086 40.024 1.00 62.82	S
ATOM 10266 CE MET F 396		C
ATOM 10267 N GLUF 397		N
ATOM 10268 CA GLU F 397		С
ATOM 10269 C GLU F 397	42.540 18.502 34.931 1.00 68.28	С
ATOM 10270 O GLU F 397	42.172 17.409 34.479 1.00 70.22	0
ATOM 10271 CB GLUF 397	44.000 17.119 36.311 1.00 75.00	С
ATOM 10272 CG GLUF 397	45.131 16.996 37.322 1.00 81.33	С
ATOM 10273 CD GLUF 397		С
ATOM 10274 OE1 GLUF 39		0
ATOM 10275 OE2 GLU F 39		0
ATOM 10276 N HIS F 398	41.743 19.522 34.719 1.00 66.05	N
ATOM 10277 CA HIS F 398	40.551 19.495 33.880 1.00 64.49	С
ATOM 10278 C HIS F 398	40.620 20.802 33.092 1.00 63.29	С

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ATOM	10369	N LEUF 410	31.667 22.577 35.902 1.00 56.56	N
		CA LEUF 410	31.244 23.545 34.902 1.00 57.26	С
		C LEUF 410	32.413 23.805 33.970 1.00 59.35	С
		O LEUF 410	33.584 23.637 34.304 1.00 58.97	0
ATOM	10373	CB LEUF 410	30.668 24.837 35.464 1.00 55.77	С
ATOM	10374	CG LEUF 410	29.667 24.528 36.601 1.00 54.83	C
		CD1 LEU F 410	29.205 25.798 37.278 1.00 55.52	С
		-	28.505 23.766 36.001 1.00 54.77	С
		N ASP F 411	31.952 24.202 32.790 1.00 62.19	N
		•••	32.831 24.505 31.661 1.00 64.49	С
		C ASP F 411	32.795 25.997 31.412 1.00 64.48	C
		O ASP F 411		O C
ATOM	10381	CB ASP F 411	32.228 23.669 30.538 1.00 68.33	C
			32.391 24.299 29.173 1.00 72.19 31.696 25.321 28.932 1.00 73.43	O
			33.220 23.750 28.392 1.00 74.63	ő
		N ARG F 412		N
			33.906 28.019 30.696 1.00 65.23	Ċ
		C ARG F 412		C
_		O ARG F 412		0
			34.982 28.444 29.689 1.00 64.44	С
ATOM	10390	CG ARG F 412	34.710 29.873 29.244 1.00 64.57	С
			35.927 30.537 28.674 1.00 65.66	С
		NE ARG F 412		N
		CZ ARG F 412		C
		NH1 ARG F 412	33.978 31.914 27.094 1.00 66.89	N
		NH2 ARG F 412	34.842 33.932 27.799 1.00 67.45	N
		N ASN F 413	32.083 28.198 29.112 1.00 68.07	N C
			30.830 28.695 28.572 1.00 70.73 29.668 28.640 29.522 1.00 70.13	c
		C ASN F 413	28.805 29.535 29.411 1.00 70.65	o
		O ASN F 413 CB ASN F 413	30.525 27.900 27.282 1.00 74.76	C
		CG ASN F 413		Č
		OD1 ASN F 413	32.005 29.230 25.952 1.00 80.28	0
		ND2 ASN F 413	32.560 27.007 26.279 1.00 79.96	N
		N GLN F 414	29,592 27.702 30.462 1.00 68.79	N
		CA GLNF 414	28.458 27.658 31.391 1.00 68.63	С
		C GLN F 414	28.438 28.884 32.296 1.00 67.98	С
		O GLN F 414	27.433 29.292 32.874 1.00 66.88	0
		CB GLN F 414	28.463 26.359 32.177 1.00 69.46	C
		CG GLN F 414	28.856 25.169 31.307 1.00 70.47	C
		CD GLN F 414	28.369 23.893 31.965 1.00 71.50	С
		OE1 GLN F 414	29.171 23.019 32.299 1.00 71.94	O N
		NE2 GLN F 414	27.044 23.864 32.118 1.00 72.39	N
ATOM	10413	N GLYF415	29.596 29.527 32.400 1.00 67.80	14

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ATOM 10414 CA GIVE 415	29.746 30.770 33.128 1.00 68.11	C
	28.777 31.750 32.470 1.00 68.30	
	28.072 32.412 33.224 1.00 68.90	
	28.604 31.849 31.163 1.00 69.39	
	27.655 32.763 30.541 1.00 70.28	C
	26.246 32.690 31.106 1.00 69.50	C
	25.479 33.656 30.958 1.00 69.84	Ō
	27.606 32.594 29.019 1.00 71.83	C
	28.968 32.338 28.420 1.00 75.31	С
	29.289 33.295 27.285 1.00 78.73	С
ATOM 10424 CE LYS F 416	29.356 32.551 25.946 1.00 81.02	С
ATOM 10425 NZ LYS F 416	30.705 31.935 25.732 1.00 82.82 25.830 31.622 31.772 1.00 68.21	N
ATOM 10426 N CYS F 417	25.830 31.622 31.772 1.00 68.21	N
	24.503 31.540 32.358 1.00 67.61	
	24.285 32.661 33.350 1.00 65.76	С
	23.207 33.256 33.316 1.00 66.11	0
	24.329 30.165 32.985 1.00 70.15	C
	24.382 28.881 31.683 1.00 77.76	
	25.241 33.005 34.210 1.00 63.55	
	25.081 34.098 35.147 1.00 61.32	
	25.746 35.372 34.665 1.00 61.63	C
	26.850 35.314 34.165 1.00 61.60	0
	25.650 33.726 36.514 1.00 60.64	C
	25.593 34.885 37.508 1.00 60.21 24.857 32.547 37.066 1.00 60.33	
	25.098 36.508 34.813 1.00 63.38	N
	25.600 37.807 34.409 1.00 65.89	
	26.960 38.096 34.988 1.00 65.05	
	27.258 37.846 36.153 1.00 65.71	Ö
	24.595 38.828 34.919 1.00 70.65	C
	24.275 39.972 33.979 1.00 77.55	Č
	23.670 41.169 34.709 1.00 81.92	Č
	22.879 40.963 35.681 1.00 84.01	0
	23.980 42.334 34.320 1.00 84.04	0
ATOM 10448 N GLY F 420	27.891 38.587 34.199 1.00 65.03	N
ATOM 10449 CA GLY F 420	29.231 38.899 34.651 1.00 65.49	С
ATOM 10450 C GLY F 420	30.119 37.823 35.225 1.00 64.82	С
ATOM 10451 O GLY F 420	31.218 38.147 35.713 1.00 65.72	O
ATOM 10452 N MET F 421	29.771 36.558 35.173 1.00 64.00	N
ATOM 10453 CA MET F 421	30.550 35.454 35.683 1.00 63.00	С
ATOM 10454 C MET F 421	31.674 34.951 34.797 1.00 61.94	C
ATOM 10455 O MET F 421	32.661 34.408 35.287 1.00 62.44	0
ATOM 10456 CB MET F 421	29.596 34.239 35.805 1.00 63.18	С
	29.044 34.224 37.212 1.00 64.57	C
ATOM 10458 SD MET F 421	30.025 33.019 38.110 1.00 66.08	S

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ATOM 10459 CE MET F 421	29.018 31.565 37.788 1.00 66.03	C
ATOM 10460 N VAL F 422	31.527 35.070 33.490 1.00 60.71	N
	32.525 34.592 32.566 1.00 60.20	C C
ATOM 10462 C VAL F 422	33.905 35.167 32.837 1.00 59.38 34.851 34.392 32.683 1.00 59.80	0
ATOM 10464 CD VALE 422	34,851 34,392 32,083 1.00 35,80	C
	32.263 34.966 31.088 1.00 61.22 32.401 33.709 30.248 1.00 62.09	C
ATOM 10465 CG1 VAL F 422		C
ATOM 10466 CG2 VAL F 422 ATOM 10467 N GLU F 423		N
	35.329 37.030 33.410 1.00 58.15	C
	35.948 36.412 34.654 1.00 55.71	c
	37.152 36.166 34.665 1.00 56.58	0
	35.309 38.524 33.613 1.00 62.78	С
ATOM 10472 CG GLU F 423	34.629 39.272 32.485 1.00 69.47	C .
ATOM 10473 CD GLU F 423	33.123 39.329 32.718 1.00 73.86	С
	32.397 38.333 32.475 1.00 74.70	
	32.674 40.423 33.171 1.00 77.46	О
	35.112 36.171 35.662 1.00 51.62	N
	35.616 35.542 36.876 1.00 48.04	С
ATOM 10478 C ILE F 424	36.031 34.137 36.507 1.00 47.89	
ATOM 10479 O ILE F 424	37.163 33.731 36.816 1.00 49.20	0
	34.548 35.642 37.941 1.00 47.10	C C
	34.390 37.143 38.225 1.00 46.33 34.879 34.872 39.201 1.00 46.61	C
ATOM 10482 CG2 ILE F 424	33,229 37,383 39,174 1.00 47,46	C
	35.222 33.408 35.755 1.00 46.83	N
	35.619 32.071 35.322 1.00 48.22	Ċ
	36.937 32.135 34.556 1.00 49.91	C
	37.853 31.316 34.702 1.00 51.00	0
ATOM 10488 CB PHE F 425	34.539 31.451 34.440 1.00 48.12	C
ATOM 10489 CG PHE F 425	33.475 30.702 35.185 1.00 49.40	С
ATOM 10490 CD1 PHE F 425	33.123 31.077 36.486 1.00 50.06	C
ATOM 10491 CD2 PHE F 425		C
ATOM 10492 CE1 PHE F 425		C
ATOM 10493 CE2 PHE F 425	31.845 28.954 35.331 1.00 50.18	C
ATOM 10494 CZ PHE F 425	31.508 29.334 36.631 1.00 50.15	C
ATOM 10495 N ASP F 426	37.069 33.148 33.702 1.00 50.26	N C
ATOM 10496 CA ASP F 426 ATOM 10497 C ASP F 426	38.270 33.298 32.906 1.00 50.96 39.485 33.438 33.783 1.00 50.47	C
ATOM 10497 C ASP F 426 ATOM 10498 O ASP F 426	40.446 32.667 33.607 1.00 51.65	0
ATOM 10498 O ASP F 426 ATOM 10499 CB ASP F 426		C
ATOM 10499 CB ASP F 426		C
ATOM 10500 CG ASI 1 426	37.484 32.592 30.431 1.00 58.15	O
ATOM 10502 OD2 ASP F 426		0
ATOM 10503 N MET F 427		N

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ATOM	10504	CA MET F 427	40.586 34.508 35.657 1.00 46.90	С
			40.857 33.207 36.403 1.00 45.52	
			41.990 32.747 36.614 1.00 44.26	
ATOM	10507	CB MET F 427	40.243 35.659 36.593 1.00 47.63	С
ATOM	10508	CG MET F 427	40.163 36.986 35.836 1.00 48.76	С
ATOM	10509	SD MET F 427	39.866 38.355 36.971 1.00 51.55	S
ATOM	10510	CE MET F 427	38.139 38.222 37.326 1.00 49.51	C
			39.755 32.543 36.808 1.00 43.33	N
			39.933 31.284 37.518 1.00 42.21	С
			40.679 30.313 36.628 1.00 43.27	
			41.685 29.742 37.071 1.00 44.04	
ATOM	10515	CB LEUF 428	38.603 30.737 37.999 1.00 40.78 38.010 31.542 39.159 1.00 40.48	C
ATOM	10516	CD LEUF 428	38.010 31.542 39.159 1.00 40.48	C
			36.570 31.132 39.363 1.00 40.58	
		N LEU F 429	38.790 31.334 40.446 1.00 40.90 40.229 30.165 35.373 1.00 43.15	N
			40.881 29.212 34.467 1.00 41.90	
			42.337 29.526 34.262 1.00 42.47	
			43.205 28.654 34.401 1.00 44.16	
			40.094 29.096 33.184 1.00 41.71	
ATOM	10524	CG LEUF 429	38.733 28.397 33.360 1.00 43.05	Č
			37.812 28.671 32.178 1.00 43.57	
ATOM	10526	CD2 LEU F 429	38.859 26.908 33.606 1.00 42.12	С
			42.669 30.773 33.988 1.00 42.24	N
			44.058 31.159 33.815 1.00 42.75	С
			44.897 30.803 35.037 1.00 45.07	
			46.075 30.391 34.916 1.00 46.71	
ATOM	10531	CB ALA F 430	44.065 32.663 33.669 1.00 43.28	C
ATOM	10532	CA TUD E 421	44.355 30.955 36.258 1.00 44.77 45.170 30.623 37.427 1.00 44.31	N C
			45.397 29.124 37.461 1.00 44.45	C
			46.471 28.610 37.767 1.00 44.16	O
			44.451 30.999 38.735 1.00 44.07	C
			43.999 32.353 38.616 1.00 43.94	
			45.396 30.809 39.903 1.00 43.20	. C
		N SER F 432	44.289 28.452 37.131 1.00 45.50	N
ATOM	10540	CA SER F 432	44.289 26.983 37.159 1.00 47.34	С
ATOM	10541	C SER F 432	45.353 26.431 36.223 1.00 47.54	С
			46.118 25.497 36.477 1.00 46.82	0
			42.903 26.432 36.839 1.00 47.98	C
			43.039 25.012 36.825 1.00 49.24	0
		N SER F 433		N
			46.357 26.804 34.038 1.00 50.63	C
		C SER F 433	47.786 27.084 34.459 1.00 51.26 48.760 26.362 34.273 1.00 50.75	C O
YI OM	10346	U SER F 433	46,700 20,302 34,273 1,00 30,73	U

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ATOM 10504 C MET E 438	54.323 23.791 37.986 1.00 62.79	С
	55.142 23.592 38.867 1.00 61 09	
	53.990 26.137 38.332 1.00 64.74	
ATOM 10597 CG MET F 438	53.772 27.547 37.812 1.00 64.81	С
ATOM 10598 SD MET F 438	54.135 28.703 39.127 1.00 67.15	S
	55.311 27.925 40.183 1.00 66.27	
ATOM 10600 N ASN F 439	53.346 22.974 37.644 1.00 63.21	N
ATOM 10601 CA ASN F 439	53.225 21.673 38.262 1.00 64.74	С
	53.320 21.799 39.773 1.00 63.07	C
	54.190 21.319 40.489 1.00 62.09	
ATOM 10605 CG ASNE 430	54.353 20.818 37.695 1.00 69.48 54.162 19.398 38.206 1.00 73.82	C C
	55.154 18.664 38.273 1.00 76.98	
	52.924 19.053 38.568 1.00 75.36	
ATOM 10608 N LEUF 440		
	52.194 22.815 41.694 1.00 59.97	C
	51.887 21.539 42.469 1.00 60.37	C
ATOM 10611 O LEU F 440	50.964 20.775 42.194 1.00 60.25	0
ATOM 10612 CB LEUF 440	51.075 23.839 41.882 1.00 58.78	С
	50.694 24.208 43.313 1.00 57.87	
	51.794 25.026 43.970 1.00 56.53	
	49.366 24.945 43.317 1.00 57.72	
	52.708 21.324 43.477 1.00 60.52	
	52.558 20.194 44.348 1.00 61.60	C C
	51.530 20.432 45.431 1.00 61.09 51.343 21.567 45.857 1.00 62.04	
	53,920 20.060 45.068 1.00 64.19	
ATOM 10621 CG GLN F 441	55.044 19.592 44.172 1.00 67.64	Č
ATOM 10622 CD GLN F 441	55.044 19.592 44.172 1.00 67.64 54.612 18.553 43.142 1.00 69.80	Ċ
ATOM 10623 OE1 GLN F 441	54.443 17.386 43.525 1.00 71.77	0
ATOM 10624 NE2 GLN F 441	54.418 18.950 41.885 1.00 69.81	N
	50.917 19.379 45.953 1.00 60.60	N
ATOM 10626 CA GLY F 442	49.963 19.503 47.043 1.00 58.41	С
ATOM 10627 C GLY F 442	50,664 20.048 48.283 1.00 57.04	C
ATOM 10628 O GLY F 442	50.017 20.830 48.990 1.00 57.25	0
ATOM 10629 N GLU F 443	51.920 19.742 48.570 1.00 55.94	N
ATOM 10630 CA GLUF 443 ATOM 10631 C GLUF 443	52.532 20.303 49.768 1.00 58.15 52.645 21.826 49.592 1.00 56.01	C C
ATOM 10631 C GLU F 443	52.528 22.584 50.556 1.00 55.68	0
	53.896 19.797 50.198 1.00 62.35	C
	54.179 18.318 50.317 1.00 66.50	Č
	53.709 17.564 49.077 1.00 69.75	Ċ
	53.997 17.966 47.916 1.00 70.12	O
ATOM 10637 OE2 GLU F 443	52.996 16.549 49.342 1.00 72.24	Ο
ATOM 10638 N GLU F 444	52.894 22.219 48.348 1.00 53.52	N

			34210	
			52.988 23.648 48.033 1.00 51.41	
			51.610 24.283 48.190 1.00 49.54	С
			51.443 25.304 48.870 1.00 49.51	Ο
			53.481 23.811 46.604 1.00 51.00	C
			54.985 23.559 46.525 1.00 50.83	С
ATOM	10644	CD GLUF 444	55.461 23.611 45.082 1.00 50.64	С
			54.717 23.092 44.219 1.00 50.76	О
ATOM	10646	OE2 GLU F 444	56.559 24.173 44.898 1.00 49.61	О
		N PHE F 445		N
			49.252 24.097 47.690 1.00 46.23	С
			48.842 24.458 49.124 1.00 47.00	С
			48.378 25.546 49.478 1.00 47.60	О
			48.288 23.052 47.176 1.00 43.41	C
ATOM	10652	CG PHE F 445	46.861 23.372 47.452 1.00 42.77	C
			46.282 24.521 46.973 1.00 43.64	С
			46.091 22.512 48.186 1.00 43.76	C
			44.951 24.813 47.212 1.00 44.82	C
			44.748 22.772 48.458 1.00 44.81	C
			44.179 23.932 47.962 1.00 45.27	C
			49.023 23.507 50.012 1.00 46.82	N
			48.660 23.616 51.425 1.00 46.58	C
			49.366 24.778 52.074 1.00 47.18	C
			48.814 25.462 52.965 1.00 47.41	0
			48.850 22.180 51.966 1.00 46.32	C
			49.788 21.987 53.122 1.00 45.59	C
			47.474 21.582 52.273 1.00 46.15	C
			50.600 25.080 51.675 1.00 46.65	N C
			51.297 26.197 52.302 1.00 48.27	C
			50.776 27.548 51.838 1.00 49.24	0
			50.649 28.497 52.611 1.00 49.40	C
ATOM	10009	CB CYS F 447	52.764 26.117 51.886 1.00 50.10 53.656 24.982 52.943 1.00 53.85	S
			50.490 27.658 50.525 1.00 48.80	N
		N LEUF 448 CA LEUF 448	49.967 28.898 49.961 1.00 46.96	C
		C LEUF 448	48.634 29.240 50.623 1.00 46.33	C
		O LEUF 448	48.356 30.354 51.071 1.00 47.24	Ö
		CB LEUF 448	49.753 28.756 48.470 1.00 46.50	C
		CG LEUF 448	50.982 28.820 47.584 1.00 46.81	Č
		CD1 LEU F 448	50.525 28.569 46.148 1.00 48.16	C
		CD2 LEU F 448	51.731 30.124 47.684 1.00 45.78	Č
		N LYS F 449	47.782 28.221 50.726 1.00 44.50	N
		CA LYS F 449	46.492 28.407 51.367 1.00 43.31	Ċ
		C LYS F 449	46.691 28.978 52.754 1.00 42.85	c
			45.996 29.937 53.119 1.00 43.25	Ö
		CB LYS F 449	45.749 27.103 51.327 1.00 43.90	C
Y I OIM	10003	CD LIST 777	15.742 27.105 51.527 1.00 15.20	•

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ΔΤΩΜ	10684	CG I YS F 449	44.247 27.263 51.191 1.00 44.78	С
ATOM	10685	CD LYS F 449	43.613 26.159 51.990 1.00 47.21	Č
ATOM	10686	CE LYS F 449	43.433 24.850 51.206 1.00 47.74	Č
ATOM	10687	NZ LYS F 449	42.589 24.020 52.170 1.00 50.18	N
			47.639 28.500 53.553 1.00 42.46	
			47.814 29.119 54.875 1.00 42.90	С
			48.383 30.521 54.786 1.00 42.09	С
			48.029 31.365 55.595 1.00 43.54	0
ATOM	10692	CB SER F 450	48.795 28.347 55.761 1.00 43.59	С
ATOM	10693	OG SER F 450	48.248 27.029 55.787 1.00 47.77	O
			49.269 30.781 53.834 1.00 40.12	N
ATOM	10695	CA ILEF 451	49.820 32.118 53.722 1.00 39.28	С
ATOM	10696	C ILE F 451	48.634 33.042 53.469 1.00 39.77 48.568 34.114 54.089 1.00 39.70	С
ATOM	10697	O ILE F 451	48.568 34.114 54.089 1.00 39.70	O
ATOM	10698	CB ILE F 451	50.814 32.179 52.553 1.00 40.03	C .
			52.019 31.314 52.972 1.00 40.96	С
ATOM	10700	CG2 ILE F 451	51.168 33.605 52.181 1.00 37.43	С
ATOM	10701	CD1 ILE F 451	53.226 31.501 52.067 1.00 42.25	С
			47.705 32.616 52.586 1.00 38.84	N
			46.548 33.463 52.283 1.00 37.28	C
ATOM	10704	C ILE F 452	45.768 33.774 53.550 1.00 38.23	
ATOM	10705	O ILE F 452	45.435 34.904 53.888 1.00 38.53 45.621 32.826 51.235 1.00 35.26	0
				С
			46.372 32.603 49.939 1.00 34.97	C
ATOM	10708	CG2 ILE F 452	44.378 33.683 51.037 1.00 34.63	C
ATOM	10709	CDI ILE F 452	45.603 32.333 48.672 1.00 34.25 45.448 32.766 54.353 1.00 39.02	N
ATOM	10/10	N LEUF 453	43.448 32.700 34.333 1.00 39.02	C
			44.689 32.962 55.568 1.00 38.90 45.422 33.935 56.465 1.00 40.48	
			44.764 34.756 57.094 1.00 41.71	
ATOM	10713	CD LEUF 453	44.488 31.644 56.342 1.00 37.90	C
			43.878 31.797 57.744 1.00 35.70	C
•		CD1 LEU F 453		C
		CD2 LEU F 453		Č
		N LEU F 454	46.738 33.818 56.596 1.00 41.92	N
		CA LEUF 454		C
		C LEUF 454	47.851 36.042 56.967 1.00 45.28	C
		O LEU F 454		0
		CB LEUF 454		C
		CG LEUF 454	48.483 32.896 58.962 1.00 43.99	С
		CD1 LEU F 454		С
		CD2 LEU F 454		С
ATOM	10726	N ASN F 455	48.106 36.198 55.670 1.00 46.34	N
ATOM	10727	CA ASN F 455	48.575 37.509 55.222 1.00 46.38	С
ATOM	10728	C ASN F 455	47.492 38.408 54.733 1.00 48.11	С

0

42.202 44.463 64.198 1.00 98.67

ATOM 10773 O PHE F 461

ATOM	10774	CB PHE F 461	45.304 43.939 63.383 1.00 94.47	С
			45.403 42.449 63.144 1.00 93.47	С
			44.247 41.711 62.949 1.00 93.23	С
ATOM	10777	CD2 PHE F 461	46.612 41.809 63.106 1.00 93.27	С
ATOM	10778	CE1 PHE F 461	44.292 40.364 62.725 1.00 93.64	С
ATOM	10779	CE2 PHE F 461	46.665 40.453 62.887 1.00 93.44	С
ATOM	10780	CZ PHE F 461	45.511 39.723 62.698 1.00 93.70	С
		N THR F 465		N
		CA THR F 465		С
		C THR F 465		С
ATOM	10784	O THR F 465	48.993 46.885 68.848 1.00127.12	0
ATOM	10785	CB THR F 465	47.529 50.024 69.364 1.00128.71	С
ATOM	10786	OG1 THR F 465	48.921 50.323 69.170 1.00129.08	O
ATOM	10787	CG2 THR F 465	47.131 50.503 70.758 1.00129.15	C
ATOM	10788	N LEU F 466	49.036 47.920 70.818 1.00124.77	N
ATOM	10789	CA LEUF 466	50.204 47.163 71.281 1.00122.08	С
ATOM	10790	C LEU F 466	49.970 45.655 71.184 1.00119.75	С
ATOM	10791	O LEU F 466	50.911 44.895 70.921 1.00119.76	Ο
ATOM	10792	CB LEUF 466	50.594 47.589 72.695 1.00122.35	С
ATOM	10796	N LYS F 467	48.732 45.190 71.374 1.00116.39	N
ATOM	10797	CA LYS F 467	48.391 43.782 71.229 1.00112.94	С
ATOM	10798	C LYS F 467	48.402 43.519 69.715 1.00108.91	С
ATOM	10799	O LYS F 467	48.770 42.432 69.289 1.00108.66	0
ATOM	10800	CB LYSF 467	47.052 43.372 71.822 1.00114.52	С
ATOM	10801	CG LYS F 467	46.877 41.889 72.158 1.00115.32	С
ATOM	10802	CD LYS F 467	45.416 41.575 72.420 1.00116.50	С
ATOM	10803	CE LYS F 467	44.993 41.530 73.881 1.00117.04	С
ATOM	10804	NZ LYS F 467	43.512 41.412 74.043 1.00116.88	N
ATOM	10805	N SER F 468	48.037 44.510 68.909 1.00103.89	N
			48.049 44.395 67.468 1.00 99.80	С
		C SER F 468	49.475 44.280 66.930 1.00 96.55	С
			49.770 43.524 66.011 1.00 96.17	O
			47.436 45.617 66.780 1.00100.03	С
		OG SER F 468	46.057 45.693 67.060 1.00101.11	0
		N LEU F 469	50.372 45.063 67.533 1.00 92.49	N
		CA LEUF 469	51.774 45.046 67.131 1.00 88.39	С
		C LEU F 469	52.313 43.664 67.458 1.00 86.07	С
		O LEU F 469	53.102 43.098 66.707 1.00 85.58	0
		CB LEUF 469	52.515 46.211 67.760 1.00 88.53	С
		N GLUF 470	51.876 43.075 68.560 1.00 83.98	N
		CA GLUF 470	52.310 41.730 68.934 1.00 82.73	С
		C GLU F 470	51.629 40.703 68.049 1.00 78.47	C
		O GLUF 470	52.219 39.715 67.627 1.00 77.03	0
		CB GLUF 470	52.114 41.561 70.419 1.00 87.19	C
ATOM	10824	CG GLUF 470	51.441 40.290 70.885 1.00 93.23	С

ATOM 11033 OG1 THR F 496 69,554 24,539 40,144 1.00 71.59 0 ATOM 11034 CG2 THR F 496 70.624 26.315 41.405 1.00 72.40 C ATOM 11035 N LEUF 497 69.504 26.377 44.115 1.00 70.17 N ATOM 11036 CA LEUF 497 69.233 27.447 45.054 1.00 71.02 C ATOM 11037 C LEUF 497 68.587 28.606 44.303 1.00 71.86 C ATOM 11038 O LEUF 497 67.750 29.339 44.829 1.00 72.92 0 ATOM 11039 CB LEUF 497 70.516 27.943 45.656 1.00 72.07 C ATOM 11040 CG LEUF 497 70.604 28.132 47.169 1.00 73.56 C C ATOM 11041 CD1 LEU F 497 71.214 29.527 47.386 1.00 74.65 C ATOM 11042 CD2 LEU F 497 69.272 28.027 47.894 1.00 73.52 68.955 28.790 43.042 1.00 72.34 ATOM 11043 N GLN F 498 N ATOM 11044 CA GLN F 498 68.370 29.836 42,221 1.00 72.36 C ATOM 11045 C GLN F 498 66.980 29.403 41.782 1.00 70.52 C ATOM 11046 O GLN F 498 66.087 30.243 41.758 1.00 71.53 0 69.221 30.186 41.003 1.00 74.85 ATOM 11047 CB GLN F 498 C ATOM 11048 CG GLN F 498 68.408 30.778 39.862 1.00 78.26 C C ATOM 11049 CD GLN F 498 69.217 31.388 38.749 1.00 80.37 ATOM 11050 OEI GLN F 498 68.953 32.513 38.305 1.00 81.97 0 ATOM 11051 NE2 GLN F 498 70.222 30.662 38.264 1.00 81.46 N ATOM 11052 N GLN F 499 66.729 28.153 41.447 1.00 68.46 N ATOM 11053 CA GLN F 499 65.380 27.771 41.038 1.00 67.58 C

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ATOM 11054 C G	LN F 499	64.432 27.889	42.225 1.00 66.81	С
ATOM 11055 O G	LN F 499	63.232 28.169	42.074 1.00 67.73	Ο
ATOM 11056 CB C	3LN F 499	65.319 26.328	40.569 1.00 68.41	С
ATOM 11057 CG C	GLN F 499	66.569 25.956	39.797 1.00 69.77	С
ATOM 11058 CD (GLN F 499	66.310 24.694	38.995 1.00 71.11	С
ATOM 11059 OE1 0	GLN F 499	66.251 23.602	39.570 1.00 72.06	0
ATOM 11060 NE2	GLN F 499	66.161 24.911	37.692 1.00 71.62	N
ATOM 11061 N G	LN F 500	65.002 27.639	43.405 1.00 64.28	N
ATOM 11062 CA C	GLN F 500	64.214 27.745	44.626 1.00 61.77	С
ATOM 11063 C G	I.N F 500	63,712 29,189	44.755 1.00 59.30	С
ATOM 11064 O G	LN F 500	62.486 29.340	44.816 1.00 58.46	0
ATOM 11065 CB (GLN F 500	65.049 27.385	45.832 1.00 62.64	С
ATOM 11066 CG (GLN F 500	65.107 25.907	46.181 1.00 64.31	С
ATOM 11067 CD (GLN F 500	66.332 25.698	47.072 1.00 65.36	С
ATOM 11068 OE1	GLN F 500	66.529 26.331	48.105 1.00 64.72	0
ATOM 11069 NE2	GLN F 500	67.187 24.783	46.622 1.00 66.80	N
ATOM 11070 N H	IS F 501	64.620 30.184 4	14.744 1.00 55.48	N
ATOM 11071 CA I	HIS F 501	64.119 31.542	44.871 1.00 53.41	C
ATOM 11072 C H	IS F 501	63.185 31.939 4	3.734 1.00 53.11	C
ATOM 11073 O H	US F 501	62.247 32.725 4	13.949 1.00 52.75	0
ATOM 11074 CB I	HIS F 501	65.178 32.569	45.105 1.00 53.16	С
ATOM 11075 CG A	HIS F 501	66.179 32.918	44.074 0.50 53.76	С
ATOM 11076 CG B	BHIS F 501	66.317 32.267	46.012 0.50 53.33	С
ATOM 11077 ND1	AHIS F 501	67.522 33.08	1 44.383 0.50 54.09	N
ATOM 11078 ND11	BHIS F 501	66.152 31.67	7 47.244 0.50 53.82	Ν
ATOM 11079 CD2	AHIS F 501	66.066 33.15	4 42.746 0.50 53.48	C
ATOM 11080 CD21 ATOM 11081 CE14	BHIS F 501	67.651 32.48	5 45.885 0.50 53.10	С
ATOM 11081 CE1A	AHIS F 501	68.181 33.392	2 43.282 0.50 54.13	C
ATOM 11082 CE1E	BHIS F 501	67.323 31.536	5 47.834 0.50 53.60	C
ATOM 11083 NE2/	AHIS F 501	67.317 33.439	9 42.276 0.50 53.75	N
ATOM 11084 NE21	BHIS F 501	68.248 32.02	1 47.025 0.50 53.22	N
ATOM 11085 N G		63.378 31.436	42.522 1.00 52.18	N
ATOM 11086 CA			41.435 1.00 52.32	С
ATOM 11087 C G			41.678 1.00 52.12	C
ATOM 11088 O G			41.667 1.00 52.45	0
ATOM 11089 CB (40.109 1.00 53.34	C
ATOM 11090 CG			39.941 1.00 54.80	C
ATOM 11091 CD			2 38.524 1.00 55.67	C
ATOM 11092 OE1			6 37.771 1.00 56.90	
ATOM 11093 NE2			3 38.189 1.00 54.54	
ATOM 11094 N A			41.957 1.00 50.60	N
ATOM 11095 CA			2 42.212 1.00 48.59	
ATOM 11096 C A			43.364 1.00 48.70	C
ATOM 11097 O A			43.219 1.00 50.52	0
ATOM 11098 CB	ARG F 503	59.831 27.858	3 42.594 1.00 47.57	С

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ATOM 11000 CG AR	GF 503 58.495 27.133 42.397 1.00 45.41	ı с
ATOM 11100 CD AR	GF 503 58.727 25.650 42.393 1.00 43.73	. C
ATOM 11101 NE AR	GF 503 57.480 24.950 42.621 1.00 44.49	N
ATOM 11102 CZ AR		
	RG F 503 57.071 24.773 40.380 1.00 44.8	3 N
	RG F 503 55.569 23.876 41.894 1.00 45.9	
ATOM 11105 N LEU		N
ATOM 11106 CA LE		
ATOM 11107 C LEU		
ATOM 11108 O LEU		
	UF 504 60.068 31.417 46.630 1.00 43.01	
ATOM 11110 CG LE	UF 504 59.490 32.000 47.927 1.00 42.00 EUF 504 58.583 31.040 48.666 1.00 39.83	
	EUF 504 60.603 32.448 48.860 1.00 41.86	
ATOM 11112 CD2 LL ATOM 11113 N ALA		•
	A F 505 58.598 34.338 43.822 1.00 43.67	
ATOM 11115 C ALA		
ATOM 11116 O ALA		
ATOM 11117 CB AL		C
ATOM 11118 N GLN	N F 506 57.605 33.000 41.985 1.00 46.09	
	N F 506 56.482 32.715 41.101 1.00 47.54	
ATOM 11120 C GLN		
	NF 506 54.155 32.773 41.499 1.00 48.55	
	N F 506 56.782 31.736 39.967 1.00 49.18	
	LNF 506 58.224 31.567 39.570 0.50 50.40	
ATOM 11124 CG BGI		
	LNF 506 58.566 30.641 38.429 0.50 51.2 LNF 506 57.033 33.378 38.036 0.50 50.5	
	ELN F 506 58.054 29.525 38.268 0.50 51.3	
	LN F 506 55.801 33.484 38.055 0.50 52.2	
ATOM 11129 NE2AG		
ATOM 11130 NE2BG		
ATOM 11131 N LEU		N
ATOM 11132 CA LE	UF 507 54.221 31.135 43.715 1.00 46.66	С
ATOM 11133 C LEU		С
ATOM 11134 O LEU		0
ATOM 11135 CB LET		
ATOM 11136 CG LE		
ATOM 11137 CD1 LE		
ATOM 11138 CD2 LE		N C
ATOM 11139 N LEU ATOM 11140 CA LEV		
ATOM 11140 CA LEU		c
ATOM 11142 O LEU		Ö
ATOM 11143 CB LET		C

49.323 38.294 38.633 0.50 39.56

C

ATOM 11188 CE1AHIS F 513

WO 98/5681	12	358/371	PCT/GB98/0170
ATOM 11234	OG SER F 518	38.735 37.915 47.496 1.00 45.68	0
		38,420 40.048 44.953 1.00 43.38	N
ATOM 11236	CA ASN F 519	37.845 41.374 45.035 1.00 44.02	C
	C ASN F 519		C
	O ASN F 519		O
		38.851 42.484 44.829 1.00 45.86	С
		39.688 42.773 46.055 1.00 48.53	С
		39.121 42.742 47.157 1.00 51.16	0
		40.990 43.040 45.963 1.00 48.02	N
	N LYS F 520		N
		35.904 41.013 41.761 1.00 45.83	С
	C LYS F 520		С
	O LYS F 520		0
		36.431 40.565 40.408 1.00 47.55	С
		37.777 41.261 40.186 1.00 50.89	С
ATOM 11249	CD LYS F 520	37.550 42.478 39.309 1.00 53.95	С
ATOM 11250	CE LYS F 520	37.920 43.797 39.979 1.00 55.93 37.231 44.935 39.276 1.00 57.57	С
ATOM 11251	NZ LYS F 520	37.231 44.935 39.276 1.00 57.57	N
ATOM 11252	N GLY F 521	35.187 38.902 42.725 1.00 44.69	N
		34.155 37.980 43.169 1.00 45.45	
ATOM 11254	C GLY F 521	33.224 38.594 44.218 1.00 45.81	С
ATOM 11255	O GLY F 521	32.026 38.349 44.012 1.00 45.23	0
	N MET F 522	33.685 39.299 45.278 1.00 45.57	N
ATOM 11257	CA MET F 522	32.694 39.798 46.202 1.00 47.31	С
ATOM 11258	C MET F 522	31.816 40.837 45.483 1.00 49.18	С
ATOM 11259	O MET F 522	30.613 40.833 45.692 1.00 49.91	0
ATOM 11260	CB MET F 522	33.025 40.561 47.446 1.00 47.45	
ATOM 11261	CG MET F 522	34.239 40.366 48.262 1.00 48.06	
		34.116 39.120 49.518 1.00 48.25	S
ATOM 11263	CE MET F 522	32.372 38.941 49.745 1.00 46.61	C
ATOM 11264	N GLU F 523	32.444 41.697 44.684 1.00 50.85	N
ATOM 11265	CA GLUF 523	31.683 42.716 43.982 1.00 51.12	С
	C GLU F 523	30.553 42.014 43.271 1.00 48.18	С
	O GLU F 523	29.417 42.444 43.411 1.00 49.34	Ο
	CB GLUF 523	32.559 43.545 43.075 1.00 57.03	С
	CG GLUF 523	33.168 44.774 43.713 1.00 64.59	С
	CD GLUF 523	32.179 45.639 44.489 1.00 69.65	С
	OE1 GLU F 523	30.933 45.541 44.261 1.00 72.29	0
	OE2 GLU F 523	32.644 46.455 45.342 1.00 71.67	0
ATOM 11273		30.802 40.937 42.580 1.00 45.64	N
	CA HIS F 524	29.774 40.185 41.887 1.00 45.52	С
ATOM 11275		28.744 39.512 42.764 1.00 45.21	С
ATOM 11276		27.553 39.541 42.510 1.00 44.38	Ο
	CB HIS F 524	30.472 39.082 41.061 1.00 45.03	C
ATOM 11278	CG HIS F 524	29.500 38.237 40.319 1.00 44.78	С

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	360/371	
	22.685 41.297 50.772 1.00 77.26	
	23.422 42.563 50.475 1.00 78.36	
ATOM 11326 N CYS F 530		N
	21.101 42.933 45.314 1.00 77.91	C C
ATOM 11328 C CYS F 530	20.033 42.629 44.301 1.00 79.45 18.859 42.955 44.490 1.00 80.76	0
	22.025 44.114 45.016 1.00 78.70	C
	22.899 44.546 46.566 0.50 80.09	S
	21.416 45.744 45.479 0.50 80.49	S
ATOM 11332 SG BC131 350 ATOM 11333 N LYS F 531		N
	19.308 41.500 42.243 1.00 83.47	C
	18.344 40.450 42.794 1.00 84.98	C
ATOM 11336 O LYS F 531	17.427 39.952 42.142 1.00 85.33	0
	20.012 40.877 41.037 1.00 83.89	C
	20.464 41.860 39.987 1.00 85.48	
	21.392 42.952 40.500 1.00 86.16	C
ATOM 11342 N ASN F 532	18.525 40.011 44.022 1.00 86.63	N
	17.721 39.005 44.675 1.00 88.09	С
ATOM 11344 C ASN F 532	17.741 37.721 43.881 1.00 86.68	С
ATOM 11345 O ASN F 532	16.719 37.247 43.442 1.00 87.53	0
ATOM 11346 CB ASN F 532	16.298 39.519 44.872 1.00 91.72	С
ATOM 11347 CG ASN F 532	16.280 40.661 45.890 1.00 95.40	С
	16.926 40.592 46.952 1.00 96.69	
	15.536 41.730 45.570 1.00 96.83	N
ATOM 11350 N VAL F 533		N
	19.066 35.885 42.925 1.00 83.72	С
	19.706 34.836 43.834 1.00 83.84	C
	19.675 33.612 43.714 1.00 84.68 20.056 36.159 41.775 1.00 83.41	0
ATOM 11354 CB VAL F 533	20.036 36.139 41.773 1.00 83.41 20.117 34.960 40.845 1.00 83.32	C C
ATOM 11355 CG1 VAL F 533		C
	20.401 35.347 44.836 1.00 83.29	N
	21.126 34.600 45.830 1.00 82.89	C
ATOM 11359 C VAL F 534	20.234 34.332 47.037 1.00 82.22	c
ATOM 11360 O VALF 534	19.628 35.241 47.588 1.00 81.06	Ō
ATOM 11361 CB VAL F 534	22.348 35.414 46.347 1.00 83.68	С
ATOM 11362 CG1 VAL F 534	23.073 34.857 47.564 1.00 83.15	С
ATOM 11363 CG2 VAL F 534	23.361 35.599 45.222 1.00 84.29	С
ATOM 11364 N PRO F 535	20.214 33.078 47.449 1.00 82.07	N
ATOM 11365 CA PRO F 535	19.508 32.614 48.609 1.00 82.06	С
ATOM 11366 C PRO F 535	20.164 33.220 49.853 1.00 82.87	С
ATOM 11367 O PROF 535	21.297 33.709 49.932 1.00 82.26	0
ATOM 11368 CB PRO F 535	19.633 31.079 48.693 1.00 81.49	С
ATOM 11369 CG PRO F 535	20.394 30.730 47.465 1.00 81.39	С
ATOM 11370 CD PRO F 535	20.953 31.980 46.818 1.00 82.12	С

			361/2/1	
ATOM	11371	N LEUF 536	19.366 33.139 50.919 1.00 84.39	N
ATOM	11372	CA LEUF 536	19.693 33.630 52.239 1.00 84.86	С
ATOM	11373	C LEUF 536	20.559 32.725 53.103 1.00 84.56	С
ATOM	11374	O LEUF 536	20.213 32.487 54.278 1.00 86.23	Ο
ATOM	11379	N TYR F 537	21.677 32.216 52.572 1.00 82.05	N
ATOM	11380	CA TYR F 537	22.533 31.381 53.423 1.00 78.76	С
ATOM	11381	C TYR F 537	23.201 32.364 54.386 1.00 76.46	С
		O TYR F 537	23.824 33.347 54.003 1.00 75.39	Ο
			23.539 30.624 52.610 1.00 79.09	С
		CG TYR F 537		С
			22.161 28.620 51.994 1.00 80.46	С
			23.145 29.868 50.237 1.00 80.42	С
ATOM	11387	CE1 TYR F 537	21.608 27.734 51.084 1.00 81.18	С
ATOM	11388	CE2 TYR F 537	22.595 28.986 49.325 1.00 81.21	С
			21.829 27.923 49.737 1.00 81.37	С
ATOM	11390	OH TYR F 537	21.273 27.056 48.831 1.00 81.44	0
ATOM	11391	N ASP F 538	23.017 32.094 55.657 1.00 74.64	N
		CA ASP F 538		С
		C ASP F 538	25.015 33.031 56.925 1.00 67.31	С
ATOM	11394	O ASP F 538	25.420 34.172 57.159 1.00 67.72	Ο
ATOM	11395	CB ASP F 538	22.992 32.264 58.048 1.00 77.42	С
ATOM	11396	CG ASP F 538	21.619 32.886 58.290 1.00 82.13	С
ATOM	11397	OD1 ASP F 538	21.513 34.116 57.981 1.00 84.34	0
ATOM	11398	OD2 ASP F 538	20.740 32.115 58.761 1.00 84.01	O
ATOM	11399	N LEUF 539	25.798 31.971 56.859 1.00 60.88	N
ATOM	11400	CA LEUF 539	27.242 32.127 57.052 1.00 55.96	С
ATOM	11401	C LEUF 539	27.850 32.885 55.890 1.00 54.96	С
ATOM	11402	O LEUF 539	28.722 33.736 56.057 1.00 55.09	О
ATOM	11403	CB LEUF 539	27.864 30.778 57.301 1.00 53.97	С
ATOM	11404	CG LEU F 539	29.311 30.610 57.718 1.00 52.16	С
ATOM	11405	CD1 LEU F 539	29.726 31.540 58.833 1.00 51.56	C
ATOM	11406	CD2 LEU F 539	29.591 29.178 58.141 1.00 51.41	С
ATOM	11407	N LEUF 540	27.395 32.629 54.677 1.00 54.03	N
ATOM	11408	CA LEUF 540	27.856 33.296 53.469 1.00 52.36	С
ATOM	11409	C LEUF 540	27.484 34.776 53.536 1.00 52.20	С
ATOM	11410	O LEUF 540	28.332 35.624 53.228 1.00 50.74	Ο
ATOM	11411	CB LEUF 540	27.303 32.610 52.216 1.00 50.90	С
ATOM	11412	CG LEUF 540	27.756 33.150 50.857 1.00 49.79	С
		CD1 LEU F 540	29.171 32.700 50.530 1.00 48.69	С
ATOM	11414	CD2 LEU F 540	26.800 32.743 49.748 1.00 48.32	С
ATOM	11415	N LEUF 541	26.270 35.143 53.967 1.00 53.14	N
		CA LEUF 541	25.963 36.582 54.029 1.00 55.03	C
ATOM	11417	C LEUF 541	26.813 37.261 55.091 1.00 54.67	С
ATOM	11418	O LEUF 541	27.143 38.445 54.954 1.00 54.78	О
ATOM	11419	CB LEUF 541	24.471 36.886 54.165 1.00 57.03	С

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ATOM 11420 CG LEHE 541	23.726 36.216 52.990 1.00 60.87	С
	22.211 36.325 53.131 1.00 62.44	
ATOM 11422 CD2 LEU F 541	24.173 36.738 51.619 1.00 61.65	С
	27.196 36.511 56.120 1.00 53.31	N
	28.033 37.046 57.171 1.00 52.38	С
ATOM 11425 C GLU F 542	29.400 37.380 56.588 1.00 51.98	C
	29.849 38.523 56.742 1.00 52.67	0
	28.154 36.038 58.284 1.00 53.28	
	28.930 36.436 59.523 1.00 54.31 28.840 35.304 60.533 1.00 55.57	
ATOM 11429 CD GLU F 542 ATOM 11430 OE1 GLU F 542	27.804 34.582 60.554 1.00 56.26	0
	29.816 35.135 61.288 1.00 56.01	Ö
	30.050 36.440 55.913 1.00 50.17	N
	31.359 36.735 55.347 1.00 49.57	C
	31.291 37.827 54.311 1.00 50.51	С
ATOM 11435 O MET F 543	32.190 38.662 54.153 1.00 50.97	0
	31.904 35.443 54.756 1.00 50.18	С
ATOM 11437 CG MET F 543	31.928 34.338 55.818 1.00 50.58	C
ATOM 11438 SD MET F 543		
	32.371 34.811 58.480 1.00 51.39	
	30.213 37.872 53.532 1.00 51.70 30.040 38.927 52.527 1.00 51.52	
	29.902 40.269 53.223 1.00 52.54	c
ATOM 11443 O LEUF 544		Ö
	28.854 38.665 51.626 1.00 50.45	
	28.403 39.709 50.627 1.00 50.36	
ATOM 11446 CD1 LEU F 544	29.428 40.045 49.555 1.00 49.79	С
	27.139 39.252 49.892 1.00 50.77	С
	29.117 40.388 54.286 1.00 55.62	N
· ·	28.960 41.663 54.963 1.00 59.04	С
ATOM 11450 C ASP F 545	30.246 42.176 55.552 1.00 58.92	C
ATOM 11451 O ASP F 545	30.473 43.375 55.517 1.00 58.35	O C
ATOM 11452 CB ASP F 545 ATOM 11453 CG ASP F 545	27.925 41.675 56.071 1.00 63.84 26.524 41.431 55.545 1.00 69.30	C
ATOM 11453 CG ASF F 545	26.272 41.517 54.303 1.00 71.71	O
ATOM 11455 OD2 ASP F 545	25.645 41.139 56.412 1.00 71.81	Ö
ATOM 11456 N ALA F 546	31.113 41.309 56.050 1.00 60.03	N
ATOM 11457 CA ALA F 546	32.383 41.737 56.626 1.00 60.35	C .
ATOM 11458 C ALA F 546	33.065 42.685 55.670 1.00 61.98	С
ATOM 11459 O ALA F 546	33.609 43.684 56.084 1.00 62.84	0
ATOM 11460 CB ALA F 546	33.278 40.553 56.892 1.00 59.78	C
ATOM 11461 N HIS F 547	33.071 42.387 54.395 1.00 65.43	N
ATOM 11462 CA HIS F 547	33.678 43.150 53.341 1.00 68.65	C
ATOM 11463 C HIS F 547 ATOM 11464 O HIS F 547	33.001 44.445 53.024 1.00 73.29 33.676 45.455 52.845 1.00 74.87	C O
ATOM 11404 U MIS F 34/	JJ.070 4J.4J JZ.04J 1.00 /4.0/	9

ATOM 11465 CB HIS F 547 ATOM 11466 CG HIS F 547 ATOM 11467 ND1 HIS F 547 ATOM 11468 CD2 HIS F 547 ATOM 11469 CE1 HIS F 547 ATOM 11469 CE1 HIS F 547 ATOM 11469 CE1 HIS F 547 ATOM 11470 NE2 HIS F 547 ATOM 11470 NE2 HIS F 547 ATOM 11471 N ARG F 548 ATOM 11471 N ARG F 548 ATOM 11472 CA ARG F 548 ATOM 11472 CA ARG F 548 ATOM 11474 CA ARG F 548 ATOM 11474 CA ARG F 548 ATOM 11475 CB ARG F 548 ATOM 11476 CG ARG F 548 ATOM 11476 CG ARG F 548 ATOM 11477 CD ARG F 548 ATOM 11476 CG ARG F 548 ATOM 11479 CZ ARG F 548 ATOM 11480 NH1 ARG F 548 ATOM 11481 NH2 ARG F 548 ATOM 11482 CA EST F 600 ATOM 11481 NH2 ARG F 548 ATOM 11480 C EST F 600 AHETATM11485 CG EST F 600 HETATM11486 CG EST F 600 HETATM11487 C4 EST F 600 HETATM11487 C4 EST F 600 HETATM11489 CG EST F 600 HETATM11490 C7 EST F 600 HETATM11491 C1 EST F 600 HETATM11490 C7 EST F 600 HETATM11500 C17 EST F 600 HETATM11500 C10 EST F 600 HETATM11	WO 98/56812	262/071	PCT/GB98/01708
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HETATM11496 C13 EST F 600 30.699 33.372 43.550 1.00 34.81 C HETATM11497 C14 EST F 600 31.919 32.864 42.761 1.00 33.93 C HETATM11498 C15 EST F 600 32.542 34.190 42.382 1.00 34.40 C HETATM11499 C16 EST F 600 31.295 34.827 41.658 1.00 35.71 C HETATM11500 C17 EST F 600 30.135 34.338 42.522 1.00 35.71 C HETATM11501 O17 EST F 600 29.277 35.383 42.960 1.00 37.33 O HETATM11502 C18 EST F 600 31.036 34.100 44.828 1.00 34.22 C HETATM11503 O HOH U 1 21.848 58.049 128.989 1.00 40.46 O HETATM11504 O HOH U 2 2.109 53.126 126.118 1.00 65.57 O HETATM11505 O HOH U 3 6.765 53.163 127.614 1.00 50.70 O HETATM11506 O HOH U 4 4.264 57.656 127.962 1.00 59.52 O HETATM11507 O HOH U 5 6.775 58.196 126.015 1.00 44.53 O HETATM11508 O HOH U 6 8.449 55.388 126.316 1.00 49.12			C
HETATM11497 C14 EST F 600 31.919 32.864 42.761 1.00 33.93 C HETATM11498 C15 EST F 600 32.542 34.190 42.382 1.00 34.40 C HETATM11499 C16 EST F 600 31.295 34.827 41.658 1.00 35.71 C HETATM11500 C17 EST F 600 30.135 34.338 42.522 1.00 35.71 C HETATM11501 O17 EST F 600 29.277 35.383 42.960 1.00 37.33 O HETATM11502 C18 EST F 600 31.036 34.100 44.828 1.00 34.22 C HETATM11503 O HOH U 1 21.848 58.049 128.989 1.00 40.46 O HETATM11504 O HOH U 2 2.109 53.126 126.118 1.00 65.57 O HETATM11505 O HOH U 3 6.765 53.163 127.614 1.00 50.70 O HETATM11506 O HOH U 4 4.264 57.656 127.962 1.00 59.52 O HETATM11507 O HOH U 5 6.775 58.196 126.015 1.00 44.53 O HETATM11508 O HOH U 6 8.449 55.388 126.316 1.00 49.12 O			
HETATM11498 C15 EST F 600 32.542 34.190 42.382 1.00 34.40 C HETATM11499 C16 EST F 600 31.295 34.827 41.658 1.00 35.71 C HETATM11500 C17 EST F 600 30.135 34.338 42.522 1.00 35.71 C HETATM11501 O17 EST F 600 29.277 35.383 42.960 1.00 37.33 O HETATM11502 C18 EST F 600 31.036 34.100 44.828 1.00 34.22 C HETATM11503 O HOH U 1 21.848 58.049 128.989 1.00 40.46 O HETATM11504 O HOH U 2 2.109 53.126 126.118 1.00 65.57 O HETATM11505 O HOH U 3 6.765 53.163 127.614 1.00 50.70 O HETATM11506 O HOH U 4 4.264 57.656 127.962 1.00 59.52 O HETATM11507 O HOH U 5 6.775 58.196 126.015 1.00 44.53 O HETATM11508 O HOH U 6 8.449 55.388 126.316 1.00 49.12 O			
HETATM11499 C16 EST F 600 31.295 34.827 41.658 1.00 35.71 C HETATM11500 C17 EST F 600 30.135 34.338 42.522 1.00 35.71 C HETATM11501 O17 EST F 600 29.277 35.383 42.960 1.00 37.33 O HETATM11502 C18 EST F 600 31.036 34.100 44.828 1.00 34.22 C HETATM11503 O HOH U 1 21.848 58.049 128.989 1.00 40.46 O HETATM11504 O HOH U 2 2.109 53.126 126.118 1.00 65.57 O HETATM11505 O HOH U 3 6.765 53.163 127.614 1.00 50.70 O HETATM11506 O HOH U 4 4.264 57.656 127.962 1.00 59.52 O HETATM11507 O HOH U 5 6.775 58.196 126.015 1.00 44.53 O HETATM11508 O HOH U 6 8.449 55.388 126.316 1.00 49.12 O			
HETATM11500 C17 EST F 600 30.135 34.338 42.522 1.00 35.71 C HETATM11501 O17 EST F 600 29.277 35.383 42.960 1.00 37.33 O HETATM11502 C18 EST F 600 31.036 34.100 44.828 1.00 34.22 C HETATM11503 O HOH U 1 21.848 58.049 128.989 1.00 40.46 O HETATM11504 O HOH U 2 2.109 53.126 126.118 1.00 65.57 O HETATM11505 O HOH U 3 6.765 53.163 127.614 1.00 50.70 O HETATM11506 O HOH U 4 4.264 57.656 127.962 1.00 59.52 O HETATM11507 O HOH U 5 6.775 58.196 126.015 1.00 44.53 O HETATM11508 O HOH U 6 8.449 55.388 126.316 1.00 49.12 O			
HETATM11501 O17 EST F 600 29.277 35.383 42.960 1.00 37.33 O HETATM11502 C18 EST F 600 31.036 34.100 44.828 1.00 34.22 C HETATM11503 O HOH U 1 21.848 58.049 128.989 1.00 40.46 O HETATM11504 O HOH U 2 2.109 53.126 126.118 1.00 65.57 O HETATM11505 O HOH U 3 6.765 53.163 127.614 1.00 50.70 O HETATM11506 O HOH U 4 4.264 57.656 127.962 1.00 59.52 O HETATM11507 O HOH U 5 6.775 58.196 126.015 1.00 44.53 O HETATM11508 O HOH U 6 8.449 55.388 126.316 1.00 49.12 O			
HETATM11502 C18 EST F 600 31.036 34.100 44.828 1.00 34.22 C HETATM11503 O HOH U 1 21.848 58.049 128.989 1.00 40.46 O HETATM11504 O HOH U 2 2.109 53.126 126.118 1.00 65.57 O HETATM11505 O HOH U 3 6.765 53.163 127.614 1.00 50.70 O HETATM11506 O HOH U 4 4.264 57.656 127.962 1.00 59.52 O HETATM11507 O HOH U 5 6.775 58.196 126.015 1.00 44.53 O HETATM11508 O HOH U 6 8.449 55.388 126.316 1.00 49.12 O			
HETATM11503 O HOH U 1 21.848 58.049 128.989 1.00 40.46 O HETATM11504 O HOH U 2 2.109 53.126 126.118 1.00 65.57 O HETATM11505 O HOH U 3 6.765 53.163 127.614 1.00 50.70 O HETATM11506 O HOH U 4 4.264 57.656 127.962 1.00 59.52 O HETATM11507 O HOH U 5 6.775 58.196 126.015 1.00 44.53 O HETATM11508 O HOH U 6 8.449 55.388 126.316 1.00 49.12 O			
HETATM11504 O HOH U 2 2.109 53.126 126.118 1.00 65.57 O HETATM11505 O HOH U 3 6.765 53.163 127.614 1.00 50.70 O HETATM11506 O HOH U 4 4.264 57.656 127.962 1.00 59.52 O HETATM11507 O HOH U 5 6.775 58.196 126.015 1.00 44.53 O HETATM11508 O HOH U 6 8.449 55.388 126.316 1.00 49.12 O			
HETATM11505 O HOH U 3 6.765 53.163 127.614 1.00 50.70 O HETATM11506 O HOH U 4 4.264 57.656 127.962 1.00 59.52 O HETATM11507 O HOH U 5 6.775 58.196 126.015 1.00 44.53 O HETATM11508 O HOH U 6 8.449 55.388 126.316 1.00 49.12 O			
HETATM11506 O HOH U 4 4.264 57.656 127.962 1.00 59.52 O HETATM11507 O HOH U 5 6.775 58.196 126.015 1.00 44.53 O HETATM11508 O HOH U 6 8.449 55.388 126.316 1.00 49.12 O			
HETATM11507 O HOH U 5 6.775 58.196 126.015 1.00 44.53 O HETATM11508 O HOH U 6 8.449 55.388 126.316 1.00 49.12 O			
HETATM11508 O HOH U 6 8.449 55.388 126.316 1.00 49.12 O			

WO 98/56812		364/371	PCT/GB98/01708
HETATM11510 O	нон и в	21.397 55.268 122.647 1.00 47.01	O
HETATM11511 O	HOHU 9	15.628 63.018 112.608 1.00 74.18	Ö
HETATM11512 O	HOH U 10	22.790 46.040 129.344 1.00 67.31	0
HETATM11513 O	HOH U 11	11.683 46.006 112.647 1.00 59.22	0
HETATM11514 O	HOH U 12	5.895 50.660 116.043 1.00 57.86	0
HETATM11515 O	HOH U 13	25.458 70.001 126.746 1.00 73.20	0
HETATM11516 O	HOH U 14	24.497 52.915 106.792 1.00 58.51	0
HETATM11517 O	HOHU 15	4.234 56.305 140.939 1.00 80.83	0
HETATM11518 O	HOH U 16	-0.519 44.076 126.320 1.00 61.66	0
HETATM11519 O	HOH U 17	21.522 51.179 128.001 1.00 63.14	Ο
HETATM11520 O		9.168 63.071 121.769 1.00 47.72	0
HETATM11521 O		4.849 54.453 123.780 1.00 82.63	0
HETATM11522 O		25.793 58.286 139.374 1.00 54.29	0
HETATM11523 O	HOH V 2	46.017 53.443 142.101 1.00 63.10	0
HETATM11524 O	HOH V 3	40.955 53.647 140.984 1.00 43.70	0
HETATM11525 O	HOH V 4	43.837 58.030 141.000 1.00 68.06	0
	HOH V 5	40.985 58.759 142.241 1.00 56.84	0
HETATM11527 O	HOH V 6	39.196 55.915 142.293 1.00 60.34	0
HETATM11528 O	HOH V 7	29.591 50.718 141.575 1.00 61.81	0
HETATM11529 O HETATM11530 O		26.441 55.674 145.979 1.00 50.62 32.078 64.181 155.641 1.00 77.73	O O
HETATM11531 O	HOH V 10	25.073 46.126 139.508 1.00 71.06	0
HETATM11531 O	HOH V 10	35.174 46.176 155.833 1.00 70.58	0
HETATM11533 O		42.188 59.305 152.020 1.00 70.34	Ö
HETATM11534 O		22.227 70.293 141.263 1.00 69.38	Ö ·
HETATM11535 O		22.931 53.579 161.506 1.00 46.74	Ö
HETATM11536 O	HOH V 15	43.418 56.241 127.560 1.00 67.10	Ö
HETATM11537 O	=	· · · · · · · · · · · · · · · · · · ·	0
HETATM11538 O			0
HETATM11539 O	HOH V 18	38.697 63.615 146.601 1.00 59.04	0
HETATM11540 O	HOH V 19	43.599 54.688 145.358 1.00 80.66	0
HETATM11541 O	HOH W 1	18.863 40.395 92.499 1.00 45.15	0
HETATM11542 O	HOHW 2	11.617 59.649 89.904 1.00 57.58	0
HETATM11543 O		14.408 55.490 90.256 1.00 43.01	0
HETATM11544 O		9.297 54.800 88.542 1.00 70.62	0
HETATM11545 O		10.264 52.765 90.951 1.00 49.19	0
HETATM11546 O		13.313 53.121 91.929 1.00 60.26	0
HETATM11547 O		22.771 48.299 94.041 1.00 50.96	0
HETATM11548 O		19.297 43.390 98.603 1.00 47.61	0
HETATM11549 O		7.386 44.992 105.654 1.00 64.21	0
HETATM11550 O		29.628 46.851 93.188 1.00 60.24	0
HETATM11551 O		21.486 58.693 106.858 1.00 74.35	0
HETATM11552 O		6.464 54.649 100.262 1.00 68.82	0
HETATM11553 O		10.584 30.801 93.898 1.00 61.92	O O
HETATM11554 O	DUD W 14	18.917 44.913 114.684 1.00 64.21	U

WO 98/56812		365/371	PCT/GB98/01708
HETATM11555 O	HOH W 15	13.984 53.633 76.434 1.00 70.54	0
HETATM11556 O	HOH W 16	17.110 66.927 90.775 1.00 62.32	0
HETATM11557 O	HOH W 17	23.687 44.599 94.346 1.00 60.73	Ο
		6.280 48.735 95.221 1.00 55.74	0
HETATM11559 O	HOH W 19	12.146 55.843 94.680 1.00 74.27	Ο
HETATM11560 O	HOH X 1		0
HETATM11561 O	HOH X 2		Ο
HETATM11562 O	HOH X 3		0
HETATM11563 O	HOH X 4		0
HETATM11564 O	HOH X 5		O
	HOH X 6	33.241 25.772 84.263 1.00 51.97	0
	HOH X 7	32.254 36.799 83.153 1.00 56.64	0
	HOH X 8		0
	HOH X 9		0
		32.682 43.133 84.366 1.00 66.26	0
		42.892 33.559 71.691 1.00 65.92	0
HETATM11571 O	HOH X 12	33.790 20.271 74.636 1.00 51.74	0 0
HETATM11572 O		12.440 31.491 79.143 1.00 57.12 31.046 37.551 62.222 1.00 52.34	0
	HOH X 14	31.421 23.945 99.377 1.00 72.53	0
	HOH X 15		0
		29.439 39.000 82.982 1.00 65.46	Ö
		27.652 21.245 79.034 1.00 41.31	Ö
		36.035 24.694 81.219 1.00 73.20	Ö
HETATM11578 O	HOH Y 1	51.022 42.856 41.650 1.00 50.42	ŏ
HETATM11580 O	HOH Y 2	55,305 63.132 43.048 1.00 53.02	Ō
HETATM11581 O	HOH Y 3		O .
	HOH Y 4	58.073 58.597 44.494 1.00 58.72	0
	HOH Y 5		0
HETATM11584 O	HOHY 6		Ο
HETATM11585 O	HOH Y 7		0
	HOHY 8	50.324 45.115 34.825 1.00 50.83	Ο
HETATM11587 O	HOHY 9	62.094 47.962 27.730 1.00 76.57	0
HETATM11588 O	HOHY 10	39.885 46.806 39.557 1.00 61.46	Ο
HETATM11589 O	HOH Y 11	46.347 59.084 26.059 1.00 72.51	Ο
HETATM11590 O	HOHY 12	61.345 58.138 33.022 1.00 56.38	Ο
HETATM11591 O	HOH Y 13	60.304 34.626 39.805 1.00 61.76	0
HETATM11592 O	HOHY 14	50.352 45.472 18.863 1.00 50.26	0
HETATM11593 O	HOH Y 15	53.818 57.125 56.560 1.00 66.19	0
	HOH Y 16	48.360 68.736 42.101 1.00 67.02	0
HETATM11595 O		45.590 45.900 38.932 1.00 68.45	0
	HOH Y 18	62.449 52.794 38.213 1.00 47.80	0
	HOH Y 19	55.536 59.041 38.868 1.00 68.17	0
	HOH Z 1	46.934 37.171 50.101 1.00 41.17	0
HETATM11599 O	HOH Z 2	34.165 20.922 47.061 1.00 50.41	О

WO 98/56812		366/371	PCT/GB98/01708
HETATM11600 O	HOHZ 3	36.863 25.565 47.746 1.00 48.74	0
HETATM11601 O	HOHZ 4	39.998 21.594 47.150 1.00 63.60	0
HETATM11602 O	HOHZ 5	40.839 23.368 49.585 1.00 52.11	0
HETATM11603 O	HOHZ 6	39.133 26.153 49.772 1.00 59.33	0
HETATM11604 O	HOHZ 7	38.468 36.961 50.477 1.00 47.17	0
HETATM11605 O	HOH Z 8	43.196 36.928 56.104 1.00 42.56	0
HETATM11606 O	HOHZ 9	46.400 26.653 65.467 1.00 78.67	0
HETATM11607 O	HOH Z 10	36.448 43.177 48.827 1.00 65.41	0
HETATM11608 O	HOH Z 11	28.492 31.879 62.192 1.00 59.52	0
HETATM11609 O	HOH Z 12	39.635 20.562 59.171 1.00 61.65	0
HETATM11610 O	HOH Z 13	58.948 35.086 54.821 1.00 69.60	0
HETATM11611 O	HOH Z 14	39.105 38.326 71.399 1.00 56.57	0
HETATM11612 O	HOH Z 15	41.408 24.364 34.260 1.00 75.94	0
HETATM11613 O	HOH Z 16	25.083 22.557 45.757 1.00 66.82	0
HETATM11614 O	HOH Z 17	40.578 39.812 50.158 1.00 75.22	0
HETATM11615 O	HOHZ 18	45.346 22.421 55.001 1.00 43.55	0
HETATM11616 O	HOH Z 19	37.459 24.933 52.629 1.00 75.18	0
END			

02-JUN-98

HEADER PROTEIN

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COMPND ERB RAL_TRIV_HM
REMARK 1 HOMOLOGY MODEL OF ESTROGEN RECEPTOR-BETA COMPLEXED
WITH RALOXIFENE.
REMARK 1 ONLY COORDINATES OF RESIDUES IN THE IMMEDIATE VICINITY
OF THE BINDING
REMARK 1 CAVITY WHICH DIFFER BETWEEN THE ALPHA AND BETA
ISOFORMS
REMARK 1 (I326V,L384M,M421I,F445Y) ARE INCLUDED IN THIS SET OF
COORDINATES.
REMARK 1
SEQRES 1
            1 RAL
SEQRES 1
            1 VAL
SEORES 1
            1 MET
            1 ILE
SEQRES 1
            1 TYR
SEQRES 1
                        -4.267 -4.115 0.855 1.00 0.00
ATOM 1 H1 RAL 600
        2 H2 RAL 600
                        6.124 -9.120 -4.735 1.00 0.00
ATOM
        3 H4 RAL 600
                        -6.508 -7.165 -8.533 1.00 0.00
ATOM
        4 C1 RAL 600 -2.209 -6.388 -1.171 1.00 35.79
ATOM
ATOM 5 C2 RAL 600 -3.022 -5.575 -0.418 1.00 35.77
        6 C3 RAL 600 -2.468 -4.551 0.315 1.00 34.88
ATOM
ATOM 7 O3 RAL 600 -3.394 -3.771 1.000 1.00 35.72
                        -1.095 -4.402 0.255 1.00 34.34
        8 C4 RAL 600
ATOM
ATOM 9 C5 RAL 600 -0.282 -5.210 -0.472 1.00 33.83
ATOM 10 S6 RAL 600 1.392 -5.345 -0.623 1.00 33.30
        11 C7 RAL 600 1.437 -6.614 -1.747 1.00 34.55
ATOM
                         2.670 -7.197 -2.336 1.00 34.77
        12 C8 RAL 600
ATOM
                         3.798 -7.361 -1.574 1.00 36.70
        13 C9 RAL 600
ATOM
        14 C10 RAL 600 4.963 -7.933 -2.060 1.00 38.09
ATOM
                         5.021 -8.329 -3.381 1.00 38.32
        15 C11 RAL 600
ATOM
                         6.202 -8.890 -3.817 1.00 42.30
        16 O11 RAL 600
ATOM
        17 C12 RAL 600 3.929 -8.159 -4.184 1.00 36.41
ATOM
        18 C13 RAL 600 2.784 -7.605 -3.624 1.00 35.52
ATOM
                         -0.876 -6.231 -1.207 1.00 33.48
        19 C14 RAL 600
ATOM
        20 C15 RAL 600 0.102 -7.018 -1.931 1.00 33.73
ATOM
                         -0.339 -8.082 -2.678 1.00 32.72
        21 C16 RAL 600
ATOM
        22 O16 RAL 600 0.055 -9.187 -2.381 1.00 33.17
ATOM
                         -1.153 -7.980 -3.865 1.00 30.87
        23 C17 RAL 600
ATOM
                         -1.626 -9.153 -4.381 1.00 31.15
        24 C18 RAL 600
ATOM
                         -2.365 -9.164 -5.566 1.00 31.63
        25 C19 RAL 600
ATOM
                         -2.556 -7.956 -6.174 1.00 33.92
        26 C20 RAL 600
ATOM
                         -2.033 -6.764 -5.671 1.00 33.20
        27 C21 RAL 600
ATOM
                         -1.320 -6.769 -4.485 1.00 31.18
        28 C22 RAL 600
ATOM
                         -3.256 -7.757 -7.343 1.00 36.78
        29 O23 RAL 600
ATOM
                         -4.531 -8.330 -7.438 1.00 37.00
        30 C24 RAL 600
ATOM
        31 C25 RAL 600 -4.788 -8.085 -8.967 1.00 36.45
ATOM
        32 N26 RAL 600 -5.683 -6.914 -9.055 1.00 35.91
ATOM
                         -6.172 -6.718 -10.396 1.00 36.09
        33 C27 RAL 600
ATOM
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34 C28 RAL 600
                         -6.807 -5.358 -10.722 1.00 36.35
ATOM
        35 C29 RAL 600
                         -5.854 -4.292 -10.160 1.00 37.35
ATOM
        36 C30 RAL 600
37 C31 RAL 600
                         -5.893 -4.476 -8.628 1.00 37.06
ATOM
                         -5.128 -5.781 -8.312 1.00 36.69
ATOM
TER
      38
          RAL 600
                        -10.374 0.336 6.860 1.00 28.80
        39 N VAL 326
ATOM
        40 CA VAL 326
                       -9.361 -0.745 6.687 1.00 29.08
ATOM
                        -10.098 -2.048 6.446 1.00 30.33
        41 C VAL 326
ATOM
                        -10.782 -2.408 7.420 1.00 31.88
        42 O VAL 326
ATOM
        43 CB VAL 326 -8.502 -0.851 7.960 1.00 0.00
ATOM
        44 CG1 VAL 326 -7.572 0.356 8.097 1.00 0.00
ATOM
        45 CG2 VAL 326
                         -9.380 -1.011 9.202 1.00 0.00
ATOM
      46 VAL 326
TER
       47 N MET 384
                         ATOM
                         0.330 -0.505 -5.954 1.00 27.46
        48 CA MET 384
ATOM
ATOM 49 C MET 384
                         1.092 0.363 -4.973 1.00 27.91
ATOM 50 O MET 384
                        1.177 -0.069 -3.819 1.00 30.10
ATOM 51 CB MET 384 1.242 -1.442 -6.767 1.00 0.00
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02-JUN-98

HEADER PROTEIN

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COMPND ERB RAL TRIV HM
REMARK 1 HOMOLOGY MODEL OF ESTROGEN RECEPTOR-BETA COMPLEXED
WITH ESTRADIOL.
REMARK 1 ONLY COORDINATES OF RESIDUES IN THE IMMEDIATE VICINITY
OF THE BINDING
REMARK 1 CAVITY WHICH DIFFER BETWEEN THE ALPHA AND BETA
ISOFORMS
REMARK 1 (1326V,L384M,M421LF445Y) ARE INCLUDED IN THIS SET OF
COORDINATES.
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SEORES 1
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(54) Title: ESTROGEN RECEPTOR CRYSTALS AND LIGANDS

(57) Abstract

Crystal comprising at least part of the ER α ligand binding domain, optionally bound to a ligand, ligands that bind to ER receptors, and methods of designing them, and a homology model of the ER β receptor.

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Int Honel Application No PCT/GB 98/01708

A. CLASSII IPC 6	CO7K14/72 CO7D333/54 CO7K14/72 CO7D333/54 CO7D409/04 CO7D417/04			C07D333/60
According to	International Patent Classification (IPC) or to be	oth national classification	on and IPC	
B. FIELDS				
Minimum do IPC 6	cumentation searched (classification system tol CO7K CO7J	lowed by classification	symbols)	
Documentat	on searched other than minimum documentation	n to the extent that suc	h documents are included in	the fields searched
Electronic da	ata base consulted during the international sear	ch (name of data base	and, where practical, search	terms used)
C. DOCUME	NTS CONSIDERED TO BE RELEVANT			
Category ⁻	Citation of document, with indication, where a	ppropriate, of the relev	ant passages	Relevant to claim No.
Y	ANSTEAD G M ET AL: "T pharmacophore: Ligand receptor binding affin and a model for the re STEROIDS, vol. 62, no. 3, March XP004057108 SAN FRANCISCO US cited in the applicati see page 285 - page 28 see page 287 - page 29	structure-esity relation ceptor bindi 1997, pages on 6 7	trogen ships ng site"	13
X Furth	ner documents are listed in the continuation of b	ox C.	X Patent family membe	rs are listed in annex.
° Special ca	tegories of cited documents :			
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Date of the	actual completion of the international search		Date of mailing of the inte	rnational search report
1	5 December 1998		11	02. 1999
Name and r	nailing address of the ISA		Authorized officer	
	European Patent Office, P.B. 5818 Patentle NL - 2280 HV Rijswijk Tel. (+31-70) 340-2040, Tx. 31 651 epo nl, Fax: (+31-70) 340-3016	aan 2	Rufet, J	

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ation) DOCUMENTS CONSIDERED TO BE RELEVANT Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
·	
EKENA K ET AL.: "Identification of amino acids in the hormone binding domain of the human estrogen receptor important in estrogen binding" JOURNAL OF BIOLOGICAL CHEMISTRY, vol. 271, no. 33, 16 August 1996, pages 20053-20059, XP002075903 US see page 20056, column 2 - page 20059, column 1	13,14
EKENA K ET AL.: "Different residues of the human estrogen receptor are involved in the recognition of structurally diverse estrogens and antiestrogens" JOURNAL OF BIOLOGICAL CHEMISTRY, vol. 272, no. 8, 21 February 1997, pages 5069-5075, XP002075904 BALTIMORE US see the whole document	13,14
BOURGUET W ET AL.: "Crystal structure of the ligand-binding domain of the human nuclear receptor RXR-alpha" NATURE., vol. 375, 1 July 1995, pages 377-382, XP002075905	1
see the whole document	6,7,52
GREENE G L ET AL: "SEQUENCE AND EXPRESSION OF HUMAN ESTROGEN RECEPTOR COMPLEMENTARY DNA" SCIENCE, vol. 231, no. 4742, 7 March 1986, pages 1150-1154, XP000611679 washington us see the whole document	1-4,55
WO 97 09348 A (KARO BIO AB) 13 March 1997 see the whole document	1-4,7,8, 56,58
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	acids in the hormone binding domain of the human estrogen receptor important in estrogen binding" JOURNAL OF BIOLOGICAL CHEMISTRY, vol. 271, no. 33, 16 August 1996, pages 20053-20059, XP002075903 US see page 20056, column 2 - page 20059, column 1 EKENA K ET AL.: "Different residues of the human estrogen receptor are involved in the recognition of structurally diverse estrogens and antiestrogens" JOURNAL OF BIOLOGICAL CHEMISTRY, vol. 272, no. 8, 21 February 1997, pages 5069-5075, XP002075904 BALTIMORE US see the whole document BOURGUET W ET AL.: "Crystal structure of the ligand-binding domain of the human nuclear receptor RXR-alpha" NATURE., vol. 375, 1 July 1995, pages 377-382, XP002075905 LONDON GB see the whole document GREENE G L ET AL: "SEQUENCE AND EXPRESSION OF HUMAN ESTROGEN RECEPTOR COMPLEMENTARY DNA" SCIENCE, vol. 231, no. 4742, 7 March 1986, pages 1150-1154, XP000611679 washington us see the whole document WO 97 09348 A (KARO BIO AB) 13 March 1997 see the whole document SEIELSTAD D A ET AL: "ANALYSIS OF THE STRUCTURAL CORE OF THE HUMAN ESTROGEN RECEPTOR LIGAND BINDING DOMAIN BY SELECTIVE PROTEOLYSIS/MASS SPECTROMETRIC ANALYSIS" BIOCHEMISTRY, vol. 34, no. 39, 1995, pages 12605-12615, XP002063749 EASTON, PA US

Inti Ional Application No
PCT/GB 98/01708

	ation) DOCUMENTS CONSIDERED TO BE RELEVANT	Indiana at the state of the sta
Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	DANIELIAN P S ET AL: "IDENTIFICATION OF A CONSERVED REGION REQUIRED FOR HORMONE DEPENDENTTRANSCRIPTIONAL ACTIVATION BY STEROID HORMONE RECEPTORS" EMBO JOURNAL., vol. 11, no. 3, March 1992, pages 1025-1033, XP000611428 EYNSHAM, OXFORD GB see the whole document	1-4,13,
A	GRESE T A ET AL.: "Structure-activity relationships of selective estrogen receptor modulators: modifications to the 2-arylbenzothiophene core of raloxifene" JOURNAL OF MEDICINAL CHEMISTRY., vol. 40, 17 January 1997, pages 146-167, XP002075906 WASHINGTON US	13,14
X	see the whole document see scheme 3, compounds 10b-e, n-s; compounds 11 b-e, n-s	28-31,45
P, X	BRZOZOWSKI A. ET AL.: "Molecular basis of agonism and antagonism in the oestrogen receptor" NATURE., vol. 389, 16 October 1997, pages 753-758, XP002075907 LONDON GB see the whole document	1-15, 52-58
Ρ,Χ	EP 0 826 683 A (LILLY CO ELI) 4 March 1998 see page 13, line 52 - page 14, line 18; page 14, line 56 -page 15, line 14; examples 1-18,21-23	28-31,45
Α	see page 14, line 18; page 25, lines13-14	46,47
P,X	EP 0 827 959 A (LILLY CO ELI) 11 March 1998 see page 20, line 11 - page 22, line 7; preparations 3 - 6; examples 1 - 4	28-31,45
X	US 4 436 748 A (ONG HELEN H ET AL) 13 March 1984 see examples 81, 82, 84, 85, 121 - 124, 129 - 132, 141 - 144	25-31,45
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Inte onal Application No PCT/GB 98/01708

	ation) DOCUMENTS CONSIDERED TO BE RELEVANT	In the state of th
Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Р,Х	EP 0 835 872 A (LILLY CO ELI) 15 April 1998 see page 6, lines 18 - 21, 26 - 31; page 8, lines 18, 19, 21, 22, 24, 25, 43 - 45, 49, 50 - 52; page 9, lines 32 - 34, 37, 38, 43 -51; page 10, lines 34, 35, 37, 38, 42	28-30,45
X	WO 95 10513 A (PFIZER ;CAMERON KIMBERLY O (US); SILVA JARDINE PAUL DA (US); LARSO) 20 April 1995 see page 21, lines 30 - 31	32-34, 59-62
X	US 4 133 814 A (JONES C DAVID ET AL) 9 January 1979 see examples 7,10	63
X	US 5 532 382 A (CARLSON DONALD G ET AL) 2 July 1996 see examples 3,8	63
X	CHARLES D. JONES ET AL.: "Antiestrogens." JOURNAL OF MEDICINAL CHEMISTRY., vol. 27, no. 8, 1984, pages 1057-1066, XP000560343 WASHINGTON US see page 1058, column 2	63
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Inte onal Application No PCT/GB 98/01708

		PC1/GB 98	701708
C.(Continua	ation) DOCUMENTS CONSIDERED TO BE RELEVANT		
Category '	Citation of document, with indication, where appropriate, of the relevant passages		Relevant to claim No.
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Inter onal application No.

PCT/GB 98/01708

lox I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)
his International Search Report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:
Claims Nos.: because they relate to subject matter not required to be searched by this Authority, namely: Remark: Although claim 53 could, at least partially, be considered as a mere presentation of information (Rule 39.1(v) PCT), and claim 54 at least partially as a computer programme (Rule 39.1(vi) PCT), the search has been carried out as far as possible in our systematic documentation. Claims Nos.: because they relate to parts of the International Application that do not comply with the prescribed requirements to such an extent that no meaningful International Search can be carried out, specifically:
Claims Nos.: because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a). Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)
This International Searching Authority found multiple inventions in this international application, as follows:
see additional sheet
As all required additional search fees were timely paid by the applicant, this International Search Report covers all searchable claims.
2. As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.
3. As only some of the required additional search fees were timely paid by the applicant, this International Search Report covers only those claims for which fees were paid, specifically claims Nos.:
4. No required additional search fees were timely paid by the applicant. Consequently, this International Search Report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:
Remark on Protest The additional search fees were accompanied by the applicant's protest. X No protest accompanied the payment of additional search fees.

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

This International Searching Authority found multiple (groups of) inventions in this international application, as follows:

1. Claims: 1-15,52-58

Crystals of ER-alpha and their use in a method for designing ligands which bind to an ER. Machine-radable storage medium capable of displaying a graphical three-dimensional representation of ER crystals. A method for evaluating the ability of a chemical to associate with an estrogen receptor employing computational means to perform a fitting operation.

2. Claims: 16-27 completely and 38,39,42,43,50,59-63 partially

Ligands for estrogen receptors. Ligands which have the general structure of formula Z. Pharmaceutical compositions containing these ligands and use thereof.

3. Claims: 28-31,37,45,51 completely and 35,36,38,39,42,43,48, 49,50,59-63 partially

As invention 2 but limited to an ER-alpha or ER-beta selective ligand, which is a 2'-,3'-,5'-,6'-substituted 2-aryl benzothiophene

4. Claims: 32-34 completely and 59-63 partially

As invention 2 but limited to an ER ligand capable of filling the hydrophobic cavity of ER-alpha

5. Claims: 35,36,48,49,59-63 partially

As invention 2 but limited to an ER-alpha or ER-beta selective ligand, which is a position 3 substituted estradiol

6. Claims: 40,41,44 completely and 42,59-63 partially

As invention 2 but limitd to an ER-beta selective ligand, which is a steroid nucleus with substitutions larger than methyl at the alpha 14, 16 or 17 positions

7. Claims: 46,47 completely and 59-63 partially

As inventon 2 but limited to an ER-alpha or ER-beta selective ligand which is a 6,3'-dihydroxybenzothiophene with substitutions larger than methyl at the R2' and/or R3' position

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